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(54) Title: CRYSTAL STRUCTURE OF BACE AND USES THEREOF

(57) Abstract: This invention is directed to the three dimensional crystal structure of Beta-site APP Cleaving Enzyme (BACE), and to the use of this structure in rational drug design methods to identify agents that may interact with active sites of BACE. Such agents may represent new therapeutics in the treatment and/or prevention of Alzheimer's Disease.

CRYSTAL STRUCTURE OF BACE AND USES THEREOF

Field of the Invention

[0001] The present invention relates to the three dimensional crystal structure of Beta-site APP Cleaving Enzyme (BACE), and to the use of this structure in rational drug design methods to identify agents that may interact with active sites of BACE. Such agents may represent new therapeutics in the treatment and/or prevention of Alzheimer's Disease.

Background of the Invention

A characteristic pathology of Alzheimer's Disease is the build up of [0002] insoluble amyloid plaques in the brain. These proteinaceous plaques are composed of a 4KDa, 42 amino acid fragment of β -Amyloid Precursor Protein (APP) and is termed Amyloid β -peptide (A β). The mechanism of A β production is hence of critical importance in understanding the onset and progress of Alzheimer's Disease. It has been shown that $A\beta$ is derived from the proteolytic cleavage of a larger protein, β -amyloid precursor protein (APP). Two enzymes are responsible for this cleavage; first, the enzyme β -secretase cleaves APP at residue 671 (770aa isoform of APP numbering) and then γ-secretase cleaves at residue 716. More recently, the novel transmembrane aspartic protease BACE has been identified as being β -secretase. This protein is now a significant target in a therapeutic approach to Alzheimer's Disease. In rare cases of Alzheimer's Disease that are hereditary (Familial Alzheimer's Disease (FAD)) the disease phenotype has been isolated to mutations in the β -Amyloid Precursor Protein. One particular cohort, the 'Swedish mutation', exhibits a double mutation at the β-secretase cleavage site.

[0003] Based upon the role of BACE in Alzheimer's Disease, the elucidation of the three-dimensional structure of BACE, as well as its site of binding with APP, would have important implications in the treatment and/or prevention of Alzheimer's Disease and similar diseases associated with the

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presence of insoluble amyloid plaques composed the 42 amino acid fragment of APP in the brain.

Summary of the Invention

[0004] The present invention provides a crystal of BACE complexed with an APP inhibitor peptide, as well as the three dimensional structure of BACE as derived by x-ray diffraction data of the BACE/APP inhibitor peptide crystal. Specifically, the three dimensional structure of BACE is defined by the structural coordinates shown in Figure 1, ± a root mean square deviation from the backbone atoms of the amino acids of not more than 1.5Å. The structural coordinates of BACE are useful for a number of applications, including, but not limited to, the visualization, identification and characterization of various active sites of BACE, and the BACE/APP inhibitor peptide complex, including the APP binding site. The active site structures may then be used to design various agents which interact with BACE, as well as BACE complexed with an APP protein or peptide, or related molecules.

[0005] The present invention is also directed to an active site of an APP binding protein or peptide, and preferably the APP peptide binding site of BACE that is elucidated and derived from the three dimensional structure of BACE as defined by the relative structural coordinates set forth in Figure 1, \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

In one embodiment of the present invention, the active site of the APP binding protein or peptide, preferably the APP peptide binding site of BACE, comprises the relative structural coordinates according to Figure 1 of residues SER71, GLY72, LEU91, ASP93, GLY95, SER96, VAL130, PRO131, TYR132, THR133, GLN134, ILE171, ILE179, ILE187, ALA188, ARG189, PRO190, TRP258, TYR259, ASP284, LYS285, ASP289, GLY291, THR292, THR293, ASN294, ARG296 and ARG368, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

[0007] In another embodiment, the active site of the APP binding protein or peptide, preferably the APP peptide binding site of BACE, comprises the

relative structural coordinates according to Figure 1 of residues LYS70, SER71, GLY72, GLN73, GLY74, TYR75, LEU91, VAL92, ASP93, THR94, GLY95, SER96, SER97, ASN98, TYR129, VAL130, PRO131, TYR132, THR133, GLN134, GLY135, LYS136, TRP137, LYS168, PHE169, PHE170, ILE171, ASN172, SER174, TRP176, GLY178, ILE179, LEU180, GLY181, ALA183, TYR184, ALA185, GLU186, ILE187, ALA188, ARG189, PRO190, ASP191, ASP192, ARG256, TRP258, TYR259, TYR283, ASP284, LYS285, SER286, ILE287, VAL288, ASP289, SER290, GLY291, THR292, THR293, ASN294, LEU295, ARG296, GLY325, GLU326, ARG368, VAL370, LYS382, PHE383, ALA384, ILE385, SER386, GLN387, SER388, SER389, THR390, GLY391, THR392, VAL393, GLY395, ALA396 and ILE447, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

[0008] The present invention further provides a method for identifying an agent that interacts with an active site of BACE. The method comprises the steps of: (a) determining a putative active site of BACE from a three dimensional model of BACE using the relative structural coordinates of Figure 1, \pm a root mean square deviation from the backbone atoms of the amino acids of not more than 1.5Å; and (b) performing various computer fitting analyses to identify an agent which interacts with the putative active site.

[0009] The present invention also provides method for identifying an agent that interacts with an active site of an APP binding protein or peptide, preferably BACE. The method comprises the steps of: (a) generating a three dimensional model of an active site of an APP binding protein or peptide using the relative structural coordinates according to Figure 1 of residues SER71, GLY72, LEU91, ASP93, GLY95, SER96, VAL130, PRO131, TYR132, THR133, GLN134, ILE171, ILE179, ILE187, ALA188, ARG189, PRO190, TRP258, TYR259, ASP284, LYS285, ASP289, GLY291, THR292, THR293, ASN294, ARG296 and ARG368, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å; and (b) designing an agent using the three dimensional model generated in step (a).

The present invention also provides another method for [0010] identifying an agent that interacts with an active site of an APP binding protein or peptide, preferably BACE. The method comprises the steps of: (a) generating a three dimensional model of an active site of an APP binding protein or peptide using the relative structural coordinates according to Figure 1 of residues LYS70, SER71, GLY72, GLN73, GLY74, TYR75, LEU91, VAL92, ASP93, THR94, GLY95, SER96, SER97, ASN98, TYR129, VAL130, PRO131, TYR132, THR133, GLN134, GLY135, LYS136, TRP137, LYS168, PHE169, PHE170, ILE171, ASN172, SER174, TRP176, GLY178, ILE179, LEU180, GLY181, ALA183, TYR184, ALA185, GLU186, ILE187, ALA188, ARG189, PRO190, ASP191, ASP192, ARG256, TRP258, TYR259, TYR283, ASP284, LYS285, SER286, ILE287, VAL288, ASP289, SER290, GLY291, THR292, THR293, ASN294, LEU295, ARG296, GLY325, GLU326, ARG368, VAL370, LYS382, PHE383, ALA384, ILE385, SER386, GLN387, SER388, SER389, THR390, GLY391, THR392, VAL393, GLY395, ALA396 and ILE447, \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å; and (b) designing an agent using the three dimensional model generated in step (a).

[0011] Finally, the present invention provides agents, and preferably inhibitors, identified using the foregoing methods. Small molecules or other agents which inhibit or otherwise interfere with the ability of BACE to cleave APP may be useful in the treatment and/or prevention of Alzheimer's Disease.

[**0012**] Additional objects of the present invention will be apparent from the description which follows.

Brief Description of the Figure

[0013] Figure 1 provides the atomic structural coordinates for BACE and the APP inhibitor peptide as derived by X-ray diffraction of a crystal of the BACE and APP inhibitor peptide complex. "Atom type" refers to the atom whose coordinates are being measured. "Residue" refers to the type of residue of which each measured atom is a part - i.e., amino acid, cofactor, ligand or solvent. The

"x, y and z" coordinates indicate the Cartesian coordinates of each measured atom's location in the unit cell (\mathring{A}). "Occ" indicates the occupancy factor. "B" indicates the "B-value", which is a measure of how mobile the atom is in the atomic structure (\mathring{A}^2).

Detailed Description of the Invention

[**0014**] As used herein, the following terms and phrases shall have the meanings set forth below:

Unless otherwise noted, "BACE" is Beta-site APP Cleaving Enzyme, and is the β -secretase enzyme that cleaves β -amyloid precursor protein (APP) at residue 671 (770aa isoform of APP numbering). After cleavage of APP by BACE, the remaining APP is cleaved at residue 716 by γ -secretase, leaving a 42 amino acid fragment of APP that is found in the proteinaceous plaques of Alzheimer's patients. The amino acid sequence of BACE preferably has the amino acid sequence deposited with Swiss Prot under accession number P56817, including conservative substitutions. As used herein, BACE also includes "BACE peptides," which are molecules having less than the complete amino acid sequence of BACE. Preferably, BACE peptides include the active site in which BACE binds to and cleaves APP. Most preferably, the BACE peptide corresponds to amino acid residues 58-447 set forth in Figure 1 ("BACE₅₈₋₄₄₇"), including conservative substitutions.

[0016] "APP" is β -amyloid precursor protein having the amino acid sequence deposited with Swiss Prot under accession number CAA31830, including conservative substitutions. As used herein, APP also includes "APP peptides," which are molecules having less than the complete amino acid sequence of APP. Preferably, APP peptides include the active site in which APP is cleaved by BACE.

[**0017**] An "APP inhibitor peptide" is a peptide which inhibits binding between BACE and APP. Preferably, the APP peptide has the amino acid sequence SER-GLU-VAL-ASN-Sta-VAL-ALA-GLU-PHE, where Sta is rare amino acid (S)-Statine.

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[0018] An "APP binding protein or peptide" is a protein or peptide that binds APP and has a APP binding site, and includes but is not limited to BACE and BACE peptides.

[0019] Unless otherwise indicated, "protein" shall include a protein, protein domain, polypeptide or peptide.

[0020] "Structural coordinates" are the Cartesian coordinates corresponding to an atom's spatial relationship to other atoms in a molecule or molecular complex. Structural coordinates may be obtained using x-ray crystallography techniques or NMR techniques, or may be derived using molecular replacement analysis or homology modeling. Various software programs allow for the graphical representation of a set of structural coordinates to obtain a three dimensional representation of a molecule or molecular complex. The structural coordinates of the present invention may be modified from the original set provided in Figure 1 by mathematical manipulation, such as by inversion or integer additions or subtractions. As such, it is recognized that the structural coordinates of the present invention are relative, and are in no way specifically limited by the actual x, y, z coordinates of Figure 1.

[0021] An "agent" shall include a protein, polypeptide, peptide, nucleic acid, including DNA or RNA, molecule, compound or drug.

[0022] "Root mean square deviation" is the square root of the arithmetic mean of the squares of the deviations from the mean, and is a way of expressing deviation or variation from the structural coordinates of BACE described herein. The present invention includes all embodiments comprising conservative substitutions of the noted amino acid residues resulting in same structural coordinates within the stated root mean square deviation.

[0023] The numbering of the amino acid residues identified in Figure 1 are based on the numbering of the full length BACE protein from the start of the signal sequence. It will be obvious to the skilled practitioner that the numbering of the amino acid residues of BACE may be different than that set forth herein or may contain certain conservative amino acid substitutions that yield the same

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three dimensional structures as those defined in Figure 1. Corresponding amino acids and conservative substitutions in other isoforms or analogues are easily identified by visual inspection of the relevant amino acid sequences or by using commercially available homology software programs (e.g., MODELLAR, MSI, San Diego, CA).

[0024] "Conservative substitutions" are those amino acid substitutions which are functionally equivalent to the substituted amino acid residue, either by way of having similar polarity, steric arrangement, or by belonging to the same class as the substituted residue (e.g., hydrophobic, acidic or basic) and includes substitutions having an inconsequential effect on the three dimensional structure of BACE, with respect to the use of this structure for the identification and design of agents which interact with BACE, for molecular replacement analyses and/or for homology modeling.

[0025] As used herein, an "active site" refers to a region of a molecule or molecular complex that, as a result of its shape and charge potential, favorably interacts or associates with another agent (including, without limitation, a protein, polypeptide, peptide, nucleic acid, including DNA or RNA, molecule, compound, antibiotic or drug) via various covalent and/or non-covalent binding forces. Preferably, the active site of BACE corresponds to the site in which BACE cleaves the APP molecule.

[0026] As such, the active site of BACE may include, for example, both the actual site in which BACE binds and cleaves APP, as well as accessory binding sites adjacent or proximal to the actual binding site that nonetheless may affect the ability of BACE to bind and cleave APP, either by direct interference with the actual site of binding or by indirectly affecting the steric conformation or charge potential of the BACE molecule and thereby preventing or reducing the ability of BACE to bind to APP at the actual binding site. As used herein, an active site also includes BACE or BACE analog residues which exhibit observable NMR perturbations in the presence of a binding ligand, such as APP or an APP peptide. While such residues exhibiting observable NMR perturbations may not necessarily be in direct contact with or immediately

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proximate to ligand binding residues, they may be critical to BACE residues for rational drug design protocols.

[**0027**] The present invention is directed to a crystallized complex of BACE and an APP inhibitor peptide that effectively diffracts X-rays for the determination of the structural coordinates of the complex. As used herein, BACE preferably corresponds to BACE₅₈₋₄₄₇ as set forth in Figure 1, with the N-terminal domain consisting of amino acid residues 58-207 shown in Figure 1, and the C-terminal domain consisting of amino acid residues 208-447 shown in Figure 1. The APP inhibitor peptide is preferably SER-GLU-VAL-ASN-Sta-VAL-ALA-GLU-PHE.

[0028] Using the crystal complex of the present invention, X-ray diffraction data can be collected by a variety of means in order to obtain the atomic coordinates of the crystallized molecule or molecular complex. With the aid of specifically designed computer software, such crystallographic data can be used to generate a three dimensional structure of the molecule or molecular complex. Various methods used to generate and refine the three dimensional structure of a crystallized molecule or molecular structure are well known to those skilled in the art, and include, without limitation, multiwavelength anomalous dispersion (MAD), multiple isomorphous replacement, reciprocal space solvent flattening, molecular replacement, and single isomorphous replacement with anomalous scattering (SIRAS).

[0029] Accordingly, the present invention also provides the three dimensional structure of BACE as derived by x-ray diffraction data of the BACE/APP inhibitor peptide crystal. Specifically, the three dimensional structure of BACE is defined by the structural coordinates shown in Figure 1, ± a root mean square deviation from the backbone atoms of the amino acids of not more than 1.5Å, preferably not more than 1.0Å, and most preferably not more than 0.5Å. The structural coordinates of BACE are useful for a number of applications, including, but not limited to, the visualization, identification and characterization of various active sites of BACE, and the BACE/APP inhibitor peptide complex, including the APP or APP peptide binding site. The active site

structures may then be used to design agents with interact with BACE, as well as BACE complexed with APP, an APP peptide or related molecules.

[0030] The present invention is also directed to an active site of an APP binding protein or peptide, preferably the APP peptide binding site of BACE, which comprises the relative structural coordinates according to Figure 1 of residues SER71, GLY72, LEU91, ASP93, GLY95, SER96, VAL130, PRO131, TYR132, THR133, GLN134, ILE171, ILE179, ILE187, ALA188, ARG189, PRO190, TRP258, TYR259, ASP284, LYS285, ASP289, GLY291, THR292, THR293, ASN294, ARG296 and ARG368, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å, more preferably not more than 1.0Å, and most preferably not more than 0.5Å.

In another preferred embodiment, the active site of an APP [0031]binding protein or peptide, preferably the APP peptide binding site of BACE, comprises the relative structural coordinates according to Figure 1 of residues LYS70, SER71, GLY72, GLN73, GLY74, TYR75, LEU91, VAL92, ASP93, THR94, GLY95, SER96, SER97, ASN98, TYR129, VAL130, PRO131, TYR132, THR133, GLN134, GLY135, LYS136, TRP137, LYS168, PHE169, PHE170, ILE171, ASN172, SER174, TRP176, GLY178, ILE179, LEU180, GLY181, ALA183, TYR184, ALA185, GLU186, ILE187, ALA188, ARG189, PRO190, ASP191, ASP192, ARG256, TRP258, TYR259, TYR283, ASP284, LYS285, SER286, ILE287, VAL288, ASP289, SER290, GLY291, THR292, THR293, ASN294, LEU295, ARG296, GLY325, GLU326, ARG368, VAL370, LYS382, PHE383, ALA384, ILE385, SER386, GLN387, SER388, SER389, THR390, GLY391, THR392, VAL393, GLY395, ALA396 and ILE447, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å, more preferably not more than 1.0Å, and most preferably not more than 0.5Å.

[0032] Another aspect of the present invention is directed to a method for identifying an agent that interacts with an active site of BACE comprising the steps of: (a) determining an active site of BACE from a three dimensional model of BACE using the relative structural coordinates of Figure 1, \pm a root mean square deviation from the backbone atoms of said amino acids of not more than

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1.5Å, more preferably not more than 1.0Å, and most preferably not more than 0.5Å; and (b) performing computer fitting analysis to identify an agent which interacts with said active site. Computer fitting analyses utilize various computer software programs that evaluate the "fit" between the putative active site and the identified agent, by (a) generating a three dimensional model of the putative active site of a molecule or molecular complex using homology modeling or the atomic structural coordinates of the active site, and (b) determining the degree of association between the putative active site and the identified agent. Three dimensional models of the putative active site may be generated using any one of a number of methods known in the art, and include, but are not limited to, homology modeling as well as computer analysis of raw data generated using crystallographic or spectroscopy data. Computer programs used to generate such three dimensional models and/or perform the necessary fitting analyses include, but are not limited to: GRID (Oxford University, Oxford, UK), MCSS (Molecular Simulations, San Diego, CA), AUTODOCK (Scripps Research Institute, La Jolla, CA), DOCK (University of California, San Francisco, CA), Flo99 (Thistlesoft, Morris Township, NJ), Ludi (Molecular Simulations, San Diego, CA), QUANTA (Molecular Simulations, San Diego, CA), Insight (Molecular Simulations, San Diego, CA), SYBYL (TRIPOS, Inc., St. Louis. MO) and LEAPFROG (TRIPOS, Inc., St. Louis, MO).

The present invention also provides a method for identifying an agent that interacts with an active site of an APP binding protein or peptide, and preferably the APP peptide binding site on BACE. The method comprises the steps of: (a) generating a three dimensional model of an active site of an APP binding protein or peptide using the relative structural coordinates according to Figure 1 of residues SER71, GLY72, LEU91, ASP93, GLY95, SER96, VAL130, PRO131, TYR132, THR133, GLN134, ILE171, ILE179, ILE187, ALA188, ARG189, PRO190, TRP258, TYR259, ASP284, LYS285, ASP289, GLY291, THR292, THR293, ASN294, ARG296 and ARG368, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å, more preferably not more than 1.0Å, and most preferably not more than 0.5Å;

and (b) designing an agent using the three dimensional model generated in step (a). In another preferred embodiment, the active site of the APP binding protein or peptide is generated using the three dimensional model defined by the relative structural coordinates according to Figure 1 of residues LYS70, SER71, GLY72, GLN73, GLY74, TYR75, LEU91, VAL92, ASP93, THR94, GLY95, SER96, SER97, ASN98, TYR129, VAL130, PRO131, TYR132, THR133, GLN134, GLY135, LYS136, TRP137, LYS168, PHE169, PHE170, ILE171, ASN172, SER174, TRP176, GLY178, ILE179, LEU180, GLY181, ALA183, TYR184, ALA185, GLU186, ILE187, ALA188, ARG189, PRO190, ASP191, ASP192, ARG256, TRP258, TYR259, TYR283, ASP284, LYS285, SER286, ILE287, VAL288, ASP289, SER290, GLY291, THR292, THR293, ASN294, LEU295, ARG296, GLY325, GLU326, ARG368, VAL370, LYS382, PHE383, ALA384, ILE385, SER386, GLN387, SER388, SER389, THR390, GLY391, THR392, VAL393, GLY395, ALA396 and ILE447, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å, more preferably not more than 1.0Å, and most preferably not more than 0.5Å.

The effect of such an agent identified by computer fitting analyses [0034] on the APP binding protein or peptide may be further evaluated by obtaining or synthesizing the agent, and contacting the identified agent with the APP binding protein or peptide in order to determine the effect the agent has on the APP binding protein or peptide. Preferably, the APP binding protein or peptide is BACE (or a BACE peptide), and the agent is a potential inhibitor of binding between BACE (or a BACE peptide) and APP (or an APP peptide). Therefore, in the preferred embodiment, the agent is contacted with BACE (or a BACE peptide) in the presence of APP (or a APP peptide), to determine the ability of the agent to inhibit binding between BACE (or the BACE peptide) and APP (or the APP peptide). Depending upon the action of the agent on the active site, the agent may act either as an inhibitor or activator of the BACE/APP binding. Assays may be performed and the results analyzed to determine whether the agent is an inhibitor (i.e., the agent may reduce or prevent binding affinity between BACE and APP), an activator (i.e., the agent may increase binding

affinity between BACE and APP), or has no effect on the interaction between BACE and APP. Agents identified using the foregoing methods, and preferably inhibitors of BACE cleavage of APP, may then be tested as therapeutics in the treatment and/or prevention of Alzheimer's Disease, and other diseases that are also characterized by the presence of the 42 amino acid fragment of APP in the proteinaceous plaques of the brain.

[0035] Various molecular analysis and rational drug design techniques are further disclosed in U.S. Patent Nos. 5,834,228, 5,939,528 and 5,865,116, as well as in PCT Application No. PCT/US98/16879, published WO 99/09148, the contents of which are hereby incorporated by reference.

[0036] Finally, the present invention is also directed to the agents, and preferably the inhibitors, identified using the foregoing methods. Such agents may be a protein, polypeptide, peptide, nucleic acid, including DNA or RNA, molecule, compound, or drug, and preferably are small molecules that effectively inhibit binding between BACE and APP or an APP peptide. Such molecules may be useful in treating, preventing or inhibiting progression of Alzheimer's Disease.

[0037] The present invention may be better understood by reference to the following non-limiting Example. The following Example is presented in order to more fully illustrate the preferred embodiments of the invention, and should in no way be construed as limiting the scope of the present invention.

Example 1

A. Methods

[0038] Cloning of Human BACE1. Human polyA+ mRNA from whole brain (Clontech) was converted to cDNA by random-priming using Thermoscript RT-PCR System, according to the manufacturer's protocol (Lifetechnologies). This cDNA was amplified by PCR using the forward and reverse primers, 5' GCTCTAGAACCCAGC ACGGCATCCGGCTG 3' (XbaI site indicated by underlined sequence; nts. 517-537 in accession no. AF190725) and 5' CCAAGCATGCGGCCGCAATAGGCTATGGTCA TGAGGGTTGAC 3' (NotI site

indicated by underlined sequence; nts. 1809-1833; bold "A" indicates additional nucleotide to permit in-frame translation of the Fc chimera; see below), respectively. PCR was accomplished using Expand Long Polymerase kit according to the manufacturer's conditions (Roche Biochemicals; buffer #3), with PCR cycling consisting of an initial denaturing step at 95°C for 3min, 30-40 cycles of denaturation at 94°C for 30sec, annealing at 65°C for 30sec, elongation at 68°C for 1min 30sec, followed by a final elongation at 68°C for 5min. The PCR products were run on a 1% agarose gel. The appropriate band was cut out of the gel, purified by Quantum Prep Freeze 'N Squeeze DNA Extraction Columns (Bio-Rad), and cloned into the SpeI/NotI sites of the mammalian expression vector, pED/Fc (Kaufman, RJ et al., 1991, Nucl. Acids. Res. 19:4485-4490).

An intermediate construct contained the honey bee meletin [0039] secretory leader fused to the the prodomain and coding region of BACE1, just upstream to the predicted transmembrane domain of BACE1 (Vassar, R. et al., 1999, Science 286:735-741). The absence of the predicted hydrophobic transmembrane domain in this construct would permit soluble secreted BACE.Fc protein to be extracted from the conditioned medium. Downstream of BACE1 was an engineered enterokinase cleavage site followed by sequence encoding the Fc portion of immunoglobulin IgG. The final construct contained the BACE1.Fc gene, flanked by SalI and EcoRI in pED/Fc, cloned into the SalI/EcoRI sites of the mammalian expression vector, pHTop, a derivative of pED, in which the majority of the adenovirus major late promoter was replaced by six repeats of a bacterial tetracycline operator (described in Gossen et al, 1992, PNAS, 89:5547-5551). Sequencing of the BACE1.Fc recombinant gene was accomplished by BigDye terminator dideoxy sequencing using an ABI3700. Sequence analyses was accomplished using DNAstar software package.

[0040] Expression of Human BACE1. The vector, pHTOP, with the BACE1.Fc insert, contains the dihydrofolate reductase gene and when introduced in the cell line CHO/A2 (see description below) functions very

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efficiently and high expressers can be selected by isolating cells surviving in high methotrexate concentrations. The CHO/A2 cell line is derived from CHO DUKX B11 (Urlaub and Chasin, 1980, PNAS USA 77:4216-4220) by stably integrating a transcriptional activator (tTA), a fusion protein between the Tet repressor and the herpes virus VP16 transcriptional domain (Gossen et al). A CHO cell line expressing extracellular BACE1. Fc was established by transfecting (lipofection) pHTopBACE1. Fc into CHO/A2 cells and selecting clones in 0.02 and 0.05 μ M methotrexate. The conditioned media from multiple clones were screened by Western blot using a (mouse) anti-human IgG. Fc HRP antibody. The same clones were also metabolically labeled with 35 S (met/cys). The best clone, determined by virtue of its high expression, was one which resulted from 0.05 μ M MTX selection and was chosen to be scaled up for roller bottle conditioned media production (4 Liters). The conditioned media was then used for purification. The expressed protein has residues 22-460 and nine extra residues at the C-terminal (an artefact from cloning and remains of the EK cleavage site).

[0041] Purification of BACE1. For the purification of BACE the 102 liters of conditioned media was used. During purification the activity of the enzyme was estimated at room temperature by continuously monitoring the fluorescent intensity for 5-10 min. at 420 nm (ext – 320 nm) Abz-Ser-Glu-Val-Asn-Leu-Asp-Ala-Glu-Phe-Arg-Dpa (Abz = Amino benzoic acid, Dpa = 9,10-diphenylanthracene) as the substrate. The reaction mixture contained 20 μ M of substrate, different amounts of enzyme in 0.5 ml of 20 mM Tris-HCl pH 8.0 and 100 mM NaCl. The concentrated material of conditioned media(1.6 l) was applied to column (2.8 x 12 cm) containing ImmunoPure Immobilized Protein A agarose (Pierce, Il, USA) equilibrated in PBS buffer. The speed of application was 2 ml/min. The column was washed with 1 litre of PBS buffer and the BACE-Fc protein was eluted by ImmunoPure IgG Elution Buffer (Pierce, Il, USA). The fractions containing protein were immediately neutralized by 1 M Tris-HCl to pH 8.0.

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[0042] The obtained protein material was treated with Enterokinase at 25°C. The ratio of BACE-Fc to Enterokinase was 3000:1 and the time of reaction was 3 hrs. The reaction was stopped by removing Enterokinase from reaction mixture by applying the protein to a column (1 x 5 cm) containing soybean trypsin inhibitor agarose (Sigma, Mo, USA) equilibrated in 20 mM Tris-HCL pH 8.0 containing 100 mM NaCl (speed was 1 ml/min). The flow through material contained BACE and cleaved Fc. Cleaved Fc was removed from BACE by flowing through a protein A column equilibrated in 20 mM Tris-HCl pH 8.0.

[0043] BACE was partially de-glycosylated using PNGase F (New England Labs., Ma, USA). 8-9 μ g of PNGase was added to 1 mg of BACE and the incubation was carried at 37° C for 16 hrs. The additional 5-6 μ g of PNGase was added to each mg of BACE and incubation was continued for another 4 hrs. The purified BACE was separated from PNGase by HPLC size-exclusion chromatography using 21.5 x 30 cm G-3000SW column (TosoHaas, Pa, USA) equilibrated in 20 mM tris-HCL pH 8.0 containing 200 mM NaCl. (Speed of elution was 3 ml/min). The purified BACE was concentrated and used for crystallization experiments.

[0044] N-terminal sequencing of purified BACE reveals a mixture of protein species, with the major sample having the processing domain cleaved and beginning at residue 47 (all numbering refers to full length BACE; accession code: A59090) and a minor sample which had not been cleaved beginning at residue 22. A smaller sample with sequence MTIAY was also detected.

[0045] Crystallization. The crystals were grown using the hanging drop vapour diffusion method. The protein was concentrated to mg/ml in 20mM Tris pH 7.5, 200mM sodium chloride. Inhibitor peptide sequence is SEVNStaVAEF, where Sta is the rare amino acid (S)-Statine. It was concentrated to 100mM in 100% DMSO and mixed with concentrated protein in a two-fold peptide excess to form the complex. 1 μ l of complex was added to 1 μ l of well solution containing 100mM Sodium Cacodylate pH6.5, 25% PEG8K, 300mM lithium sulphate. Plate-like crystal clusters grew within one week to dimensions of 200

 μ m x 400 μ m x 75 μ m. Single crystals were transferred to a stabilizing, cryoprotectant solution which contained the well solution plus 25% Glycerol for a brief, 10 second, soak and then frozen in liquid nitrogen. X-ray diffraction crystals had space group I222, and unit cell parameters a=86.627, b=130.861, c=130.729, and α = β = γ =90°.

B. Results

Expressed in CHO cells as a fc fusion protein and, after purification, cleavage and partial deglycosylation, complexed with peptide inhibitor and crystallized. Crystals diffracted to 2.3Å and the structure was solved using the technique of molecular replacement. The search model used was derived from cod atlantic Pepsin and contained 63% of the final number of atoms. The density modified maps obtained using a poly-alanine version of the search model (39% of the final atoms) provided sufficient information to build all but 12 amino acids. The final model contains residues from 59 to 448 (using full length numbering), all 9 residues of the statine inhibitor and 360 water molecules. Of the four predicted N-linked glycosylation sites only two have interpretable electron density.

[0047] The overall shape of the BACE protein is spherical and is composed of two distinct domains, an N-terminal (58-207) and a C-terminal (208-447). With the first thirteen amino acids (58-71) being packed against residues 238-243. There is a significant cleft-like channel across one surface of the interface between the domains. This contains the inhibitor peptide and conserved aspartic acid motifs that define the active sites of aspartic proteases.

[0048] The N-terminal domain is composed of a single a-helix preceeding the loop joining the two domains and thirteen β -strands. The larger C-terminal domain has a total of seventeen β -strands and three α -helices. The overall topology is characterised by an eight stranded antiparallel interdomain β -sheet. This central sheet comprises the majority of the active site residues including the two conserved aspartates (one from each domain:93 and 289). Asp93 and

Asp289 define the position of a pseudo two-fold axis for the central β -sheet. Outside of this symmetry the two domains differ significantly. The N-terminal domain has an extra two strands extending the central sheet. In addition, there are two anti-parallel β -sheets above and below the central sheet composed of three and four β -strands respectively. Residues from the upper sheet (131-135) fold over the active site aspartates and form a 'flap' over the centre of the peptide binding cleft.

[0049] The C-terminal domain contains two lobes in addition to the strands which from the central β -sheet. These are weakly homologous to known aspartic protease structures. The binding pocket for the P1`and P3`positions are instead derived from three β -turns 388-391, 284-286 and 255-261.

[0050] There are a total of six cysteine residues in BACE. Each of these is involved in a disulphide interaction. The pattern of disulphide crosslinking, Cys278-Cys443, Cys380-Cys330, Cys420-Cys216 are unique in the aspartic proteases known to date.

[0051] A novel aspartic protease. The first attempts to study the relationship of function to structure of an Apartic proteases began in the 1930s with Pepsin. Since then this rich field of research has been successfully applied to the design of clinically used inhibitors in only one system; HIV protease. The reasons for this are related more to the validity of the pharmacological target than the efficacy of inhibitors. β -secretase has been described as a novel protease and has been shown to be linked to the onset and progression of Alzheimer's disease.

[0052] From a gross viewpoint the overall fold and domain organization is very similar to that of a canonical aspartic protease. The comparison at a more detailed level reveals a significant number of differences. The active site is characterized by two aspartic residues surrounded by a conserved set of hydrogen bonds termed a 'fireman's grip'. This is reproduced in the -secretase structure presented here. The characteristic flap which wraps over the active site in pepsin is absent from the C-terminal domain in a manner analogous to

cathepsin D. In β -secretase the critical main chain amide hydrogen bond to the carboxyl group of statine is maintained by Thr133 from this flap. The amide of the statine makes a hydrogen bond to the carboxyl group of Gly95, emphasizing that the statine residue occupies both the P1 and P1` position.

Enzyme Mechanism. It has been shown that β -secretase cleavage [0053] is dependent on proximity to the cell membrane. Both β -secretase and its substrate APP have putative transmembrane regions. Our expressed BACE construct finishes one amino acid before the predicted transmembrane region. The final residue in the current structure is Ile447, thirteen residues away from the beginning of the putative transmembrane domain. In the current crystal structure Ile447 is only 6Å away from the P3 Glutamic acid of the inhibitor suggesting a role for the remaining C-terminal residues in the enzyme mechanism. The Statine residue of the inhibitor peptide is bound at the S1 position within the active site. The position of the C-3 hydroxyl group, coplanar to and within hydrogen bonding distance of both aspartate 93 and 289 carboxyl groups, confirms that the rare amino acid mimics the tetrahedral transition state i.e the intermediate of peptide-bond hydrolysis. The distance between the oxygen atoms of Asp93 and Asp289 is 2.8Å, strongly suggesting a shared proton atom and a classic aspartic protease pK profile for these side-chains and a common enzyme mechanism to other known aspartic proteases.

Inhibitor binding. The inhibitor peptide binds in an extended form along a 20Å groove formed at the interface between the domains. The conserved catalytic aspartic residues lie at the middle of this groove. The bound peptide consists of 8 amino acids plus a statine amino acid at position 5. There is contiguous electron density for the whole peptide. The statine based inhibitor used in this study has been show to inhibit the β -secretase enzyme with nanomolar efficiency. The peptide sequence is based on the P10 to P4` APP751 Sweedish family mutation. This mutation of a Lys-Asn at the P2 position and Met-Leu at the P1 position is strongly correlated to the early onset of

Alzheimer's disease. The inhibitor peptide utilizes Statine's Leucyl like side-chain to explore this interaction. Due to the di-peptide nature of Satine the P1' position of the substrate is shifted to P2' leaving an empty S1' pocket. The β -secretase enzyme appears to have a novel preference for an apartate or glutamate at the P1' position whereas other aspartic proteases show a preference for hydrophobic residues. This unusual preference for a negatively charged P1' amino acid is explained by the guanadinium group of Arg189 forming part of the putative S1' pocket. Even at the acidic pH optima of BACE the arginine side chain would form a positively charged environment for the possibly protonated carboxyl side-chain atoms.

[0055] The S1 and S3 binding pockets are a contiguous, hydrophobic pocket formed by the side-chain of residues Tyr132, Phe169, Ile171, Trp176, Ile179 and main chain atoms of Gly74, and Gln73. This packing of inhibitor P1 and P3 side chains has been seen in previous aspartic protease complexes.

[0056] The canonical APP cleavage site for b-secretase appears to have a preference for a small hydrophobic residues at the P2` position. The side chain of the valine residue bound in the putative S2` site of β -secretase appears to not make any significant interactions with the protein, its main chain however forms a tight set of hydrogen bonds to the backbone carboxyl of Gly 95 and the sidechain OH of Tyr259. In turn, Tyr259 is held rigidly in place by an edge-pi interaction with Trp258, which packs against the guanadinium group of Arg256.

[0057] Swedish mutation. Autosomal dominant mutations identified on the β -amyloid precusor protein have been correlated to early-onset cases of Alzheimer's disease. These have been shown to cluster around the three canonical cleavage sites. A double (the so-called Swedish) mutation of Lys670-Met671 (770aa isoform of APP numbering) to Asn-Leu causes an increase in the overall quantity of $A\beta$ detectable in the plasma and in the medium of cultured fibroblasts from carriers of the Swedish mutation. These two amino acids lie at the P2 and P1 positions of the β -secretase active site. The statine based inhibitor used here is based on this Swedish mutation. A methionine at position

P1 would clearly be accommodated but would loose the van Der Waal's complentarity exhibited by the statine side-chain to Leu90 and Ile178. The C6 atom of the methione would make supplement the hydrophobic interaction to Phe169.

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Table 1

Residues of BACE Within 4Å of Peptide Inhibitor SER71, GLY72, LEU91, ASP93, GLY95, SER96, VAL130, PRO131, TYR132, THR133, GLN134, ILE171, ILE179, ILE187, ALA188, ARG189, PRO190, TRP258, TYR259, ASP284, LYS285, ASP289, GLY291, THR292, THR293, ASN294, ARG296, ARG368

Residues of BACE Within 8Å of Peptide Inhibitor
LYS70, SER71, GLY72, GLN73, GLY74, TYR75, LEU91, VAL92, ASP93, THR94,
GLY95, SER96, SER97, ASN98, TYR129, VAL130, PRO131, TYR132, THR133,
GLN134, GLY135, LYS136, TRP137, LYS168, PHE169, PHE170, ILE171,
ASN172, SER174, TRP176, GLY178, ILE179, LEU180, GLY181, ALA183,
TYR184, ALA185, GLU186, ILE187, ALA188, ARG189, PRO190, ASP191,
ASP192, ARG256, TRP258, TYR259, TYR283, ASP284, LYS285, SER286,
ILE287, VAL288, ASP289, SER290, GLY291, THR292, THR293, ASN294,
LEU295, ARG296, GLY325, GLU326, ARG368, VAL370, LYS382, PHE383,
ALA384, ILE385, SER386, GLN387, SER388, SER389, THR390, GLY391,
THR392, VAL393, GLY395, ALA396, ILE447

[0058] All publications mentioned herein above, whether to issued patents, pending applications, published articles, deposited sequences, or otherwise, are hereby incorporated by reference in their entirety. While the foregoing invention has been described in some detail for purposes of clarity and understanding, it will be appreciated by one skilled in the art from a reading of the disclosure that various changes in form and detail can be made without departing from the true scope of the invention in the appended claims.

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What is claimed is:

A crystallized complex of Beta-site APP Cleaving Enzyme
 (BACE) and SER-GLU-VAL-ASN-Sta-VAL-ALA-GLU-PHE.

- 2. The crystallized complex of Claim 1, wherein BACE has an N-terminal domain consisting of amino acid residues 58-207 shown in Figure 1, and a C-terminal domain consisting of amino acid residues 208-447 shown in Figure 1.
- 3. An active site of an APP binding protein or peptide comprising the relative structural coordinates according to Figure 1 of residues SER71, GLY72, LEU91, ASP93, GLY95, SER96, VAL130, PRO131, TYR132, THR133, GLN134, ILE171, ILE179, ILE187, ALA188, ARG189, PRO190, TRP258, TYR259, ASP284, LYS285, ASP289, GLY291, THR292, THR293, ASN294, ARG296 and ARG368, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.
- 4. The active site of Claim 3, wherein the \pm a root mean square deviation from the backbone atoms of said amino acids is not more than 1.0Å.
- 5. The active site of Claim 3, wherein the \pm a root mean square deviation from the backbone atoms of said amino acids is not more than 0.5Å.
- 6. An active site of an APP binding protein or peptide comprising the relative structural coordinates according to Figure 1 of residues LYS70, SER71, GLY72, GLN73, GLY74, TYR75, LEU91, VAL92, ASP93, THR94, GLY95, SER96, SER97, ASN98, TYR129, VAL130, PRO131, TYR132, THR133, GLN134, GLY135, LYS136, TRP137, LYS168, PHE169, PHE170, ILE171,

ASN172, SER174, TRP176, GLY178, ILE179, LEU180, GLY181, ALA183, TYR184, ALA185, GLU186, ILE187, ALA188, ARG189, PRO190, ASP191, ASP192, ARG256, TRP258, TYR259, TYR283, ASP284, LYS285, SER286, ILE287, VAL288, ASP289, SER290, GLY291, THR292, THR293, ASN294, LEU295, ARG296, GLY325, GLU326, ARG368, VAL370, LYS382, PHE383, ALA384, ILE385, SER386, GLN387, SER388, SER389, THR390, GLY391, THR392, VAL393, GLY395, ALA396 and ILE447, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

- 7. The active site of Claim 6, wherein the \pm a root mean square deviation from the backbone atoms of said amino acids is not more than 1.0Å.
- 8. The active site of Claim 6, wherein the \pm a root mean square deviation from the backbone atoms of said amino acids is not more than 0.5Å.
- 9. A method for identifying an agent that interacts with an active site of Beta-site APP Cleaving Enzyme (BACE), comprising the steps of:
- (a) determining an active site of BACE from a three dimensional model of BACE using the relative structural coordinates of Figure 1, \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 \AA ; and
- (b) performing computer fitting analysis to identify an agent which interacts with said active site.
- The method of Claim 9, wherein the \pm a root mean square deviation from the backbone atoms of said amino acids is not more than 1.0Å.
- 11. The method of Claim 9, wherein the \pm a root mean square deviation from the backbone atoms of said amino acids is not more than 0.5Å.

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- 12. A method for identifying an agent that interacts with an active site of an APP binding protein or peptide, comprising the steps of:
- (a) generating a three dimensional model of an active site of an APP binding protein or peptide using the relative structural coordinates according to Figure 1 of residues SER71, GLY72, LEU91, ASP93, GLY95, SER96, VAL130, PRO131, TYR132, THR133, GLN134, ILE171, ILE179, ILE187, ALA188, ARG189, PRO190, TRP258, TYR259, ASP284, LYS285, ASP289, GLY291, THR292, THR293, ASN294, ARG296 and ARG368, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å; and
- (b) designing an agent using the three dimensional model generated in step (a).
- 13. The method of Claim 12, wherein the \pm a root mean square deviation from the backbone atoms of said amino acids is not more than 1.0Å.
- 14. The method of Claim 12, wherein the \pm a root mean square deviation from the backbone atoms of said amino acids is not more than 0.5Å.
- 15. The method of Claim 12, wherein the agent is designed by performing computer fitting analysis of the agent with the three dimensional model generated in step (a).
- 16. The method of Claim 12, further comprising the steps of: (c) obtaining or synthesizing the agent so designed; and (d) contacting the agent with the APP binding protein or peptide in order to determine the effect the agent has on the APP binding protein or peptide.

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- 17. The method of Claim 12, wherein the APP binding protein or peptide is BACE.
- 18. The method of Claim 17, wherein the agent is a potential inhibitor of binding between BACE and APP.
- 19. The method of Claim 18, further comprising the steps of: (c) obtaining or synthesizing the agent so designed; and (d) contacting the agent with BACE in the presence of APP.
- 20. A method for identifying an agent that interacts with an active site of an APP binding protein or peptide, comprising the steps of:
- (a) generating a three dimensional model of an active site of an APP binding protein or peptide using the relative structural coordinates according to Figure 1 of residues LYS70, SER71, GLY72, GLN73, GLY74, TYR75, LEU91, VAL92, ASP93, THR94, GLY95, SER96, SER97, ASN98, TYR129, VAL130, PRO131, TYR132, THR133, GLN134, GLY135, LYS136, TRP137, LYS168, PHE169, PHE170, ILE171, ASN172, SER174, TRP176, GLY178, ILE179, LEU180, GLY181, ALA183, TYR184, ALA185, GLU186, ILE187, ALA188, ARG189, PRO190, ASP191, ASP192, ARG256, TRP258, TYR259, TYR283, ASP284, LYS285, SER286, ILE287, VAL288, ASP289, SER290, GLY291, THR292, THR293, ASN294, LEU295, ARG296, GLY325, GLU326, ARG368, VAL370, LYS382, PHE383, ALA384, ILE385, SER386, GLN387, SER388, SER389, THR390, GLY391, THR392, VAL393, GLY395, ALA396 and ILE447, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å; and
- (b) designing an agent using the three dimensional model generated in step (a).
- 21. The method of Claim 18, wherein the \pm a root mean square deviation from the backbone atoms of said amino acids is not more than 1.0Å.

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- 22. The method of Claim 20, wherein the \pm a root mean square deviation from the backbone atoms of said amino acids is not more than 0.5Å.
- 23. The method of Claim 20, wherein the agent is designed by performing computer fitting analysis of the agent with the three dimensional model generated in step (a).
- 24. The method of Claim 20, further comprising the steps of: (c) obtaining or synthesizing the agent so designed; and (d) contacting the agent with the APP binding protein or peptide in order to determine the effect the agent has on the APP binding protein or peptide.
- 25. The method of Claim 20, wherein the APP binding protein or peptide is BACE.
- 26. The method of Claim 25, wherein the agent is a potential inhibitor of binding between BACE and APP.
- 27. The method of Claim 26, further comprising the steps of: (c) obtaining or synthesizing the agent so designed; and (d) contacting the agent with BACE in the presence of APP.
 - 28. An agent identified by the method of Claim 9.
 - 29. An agent identified by the method of Claim 12.
 - 30. An agent identified by the method of Claim 20.

Figure 1

		Ator	n <u>Res</u>	<u>.</u>		X	<u>¥</u> .	$\underline{\mathbf{z}}$	
» mov	•	Type	9 -CT V	7	58	31.563	49.775	16.324	1.00 59.33
MOTA	1	7.4	GLI		58	32.861	50.358	16.764	1.00 58.44
ATOM	2	CA	GLY		58	33.594	49.446	17.727	1.00 57.81
ATOM	3	C	GLY		58	34.067	48.331	17.727	1.00 56.66
ATOM	4	0	GLY		59	33.712	49.888	18.975	1.00 56.66
ATOM	5	N	SER		59	34.391	49.094	20.015	1.00 55.45
ATOM	6	CA	SER		59	33.560	49.088	21.293	1.00 53.43
ATOM	7	C	SER		59 59	32.978	50.147	21.704	1.00 54.40
ATOM	8	0	SER		59	35.781	49.668	20.309	1.00 55.79
ATOM	9	CB OG	SER SER		59 59	35.690.		20.899	1.00 57.07
MOTA	10		PHE		60	33.480	47.924	21.927	1.00 49.96
ATOM	11	N			60	32.719	47.772	23.181	1.00 45.72
ATOM	12 13	CA C	PHE		60	33.681	47.269	24.247	1.00 44.79
ATOM			PHE		60	33.495	46.160	24.831	1.00 45.45
MOTA	14 15	O CB	PHE		60	31.564	46.790	22.976	1.00 43.28
ATOM	16	CG	PHE		60	30.557	47.249	21.957	1.00 41.00
ATOM		CD1			60	30.875	47.267	20.602	1.00 40.54
ATOM	17	CD2			60	29.301	47.701	22.355	1.00 40.58
MOTA	18				60	29.954	47.731	19.658	1.00 39.88
MOTA	19		PHE		60	28.375	48.166	21.419	1.00 39.50
ATOM	20	CE2			60	28.704	48.182	20.070	1.00 39.23
ATOM	21	CZ	PHE		61	34.709	48.073	24.500	1.00 43.29
ATOM	22	N	VAL			35.763	47.756	25.483	1.00 43.19
MOTA	23	CA	VAL		61 61	35.763	47.069	26.738	1.00 41.81
ATOM	24	C	VAL		61	35.876	46.099	27.247	1.00 42.54
MOTA	25	0				36.532	49.035	25.895	1.00 42.54
MOTA	26	CB	VAL		61 61	37.069	49.730	24.655	1.00 44.38
MOTA	27		VAL		61 61	35.621	49.975	26.676	1.00 44.28
ATOM	28		VAL			34.114	47.542	27.252	1.00 40.86
ATOM	29	N	GLU		62	33.517	46.959	28.470	1.00 40.00
ATOM	30	CA	GLU		62 62	33.208	45.473	28.320	1.00 36.45
ATOM	31	C	GLU		62	33.366	44.685	29.301	1.00 36.49
ATOM	32	0	GLU		62 62	32.226	47.700	28.832	1.00 43.76
ATOM	33 34	CB CG	GLU		62 62	32.399	48.895	29.764	1.00 48.74
MOTA	35	CD	GLU		62	32.743	48.486	31.188	1.00 51.91
ATOM	36	OE1			62	32.743	47.387	31.612	1.00 53.41
ATOM	37	OE2			62	33.423	49.271	31.890	1.00 53.64
ATOM	38	N	MET		63	32.780	45.062	27.129	1.00 30.86
ATOM ATOM	39	CA	MET		63	32.421	43.643	26.896	1.00 27.79
	40	C	MET		63	33.491	42.741	26.279	1.00 26.02
ATOM	41	0	MET		63	33.354	41.476	26.310	1.00 25.25
ATOM	42	CB	MET		63	31.130		26.078	1.00 25.63
ATOM	43	CG	MET		63	29.942	44.133	26.858	1.00 24.89
ATOM ATOM	44	SD	MET		63	28.392	44.180	25.960	1.00 23.85
ATOM	45	CE	MET		63	28,431	45.848	25.316	1.00 24.18
ATOM	46	N	VAL		64	34.551	43.330	25.736	1.00 23.39
ATOM	47	CA	VAL		64	35.639	42.516	25.143	1.00 20.76
ATOM	48	C	VAL		64	36.263	41.634	26.216	1.00 20.06
ATOM	49	Ö	VAL		64	36.531	42.095	27.370	1.00 18.87
ATOM	50	СВ	VAL		64	36.740	43.407	24.517	1.00 21.16
ATOM	51		VAL		64	37.958	42.567	24.151	1.00 18.99
	52		VAL		64	36.193	44.092	23.266	1.00 21.01
ATOM	52 53	N N	ASP		65	36.487	40.373	25.869	1.00 18.21
MOTA		CA	ASP		65	37.091	39.397	26.800	1.00 18.56
MOTA	54 55	CA	ASP		65	36.280	39.174	28.071	1.00 17.80
MOTA	55 56	0	ASP		65	36.869	38.964	29.165	1.00 16.29
ATOM	56 57	CB	ASP		65	38.508	39.829	27.194	1.00 21.53
MOTA			ASP		65	39.409	40.055	25.993	1.00 22.65
MOTA	58	CG	ಗಾಗ	A	0.5	33.403	40.000	,,,,	

				_			20 454	04 000	75
MOTA	59	OD1	ASP		65	39.162	39.451	24.930	1.00 23.75
ATOM	60	OD2	ASP	Α	65	40.375	40.831	26.117	1.00 24.72
ATOM	61	N	ASN	Α	66	34.955	39.209	27.969	1.00 16.59
ATOM	62	CA	ASN		66	34.090	38.987	29.156	1.00 16.58
			ASN		66	33.719	37.508	29.274	1.00 17.20
ATOM	63	C							
ATOM	64	0	ASN		66	32.815	37.125	30.070	1.00 19.23
ATOM	65	CB	ASN	Α	66	32.817	39.845	29.059	1.00 14.62
ATOM	66	CG	ASN	Α	66	31.967	39.516	27.835	1.00 15.57
ATOM	67	OD1	ASN	A	66	32.381	38.714	26.937	1.00 16.31
ATOM	68		ASN		66	30.788	40.120	27.760	1.00 14.85
	69		LEU		67	34.409	36.664	28.515	1.00 17.73
MOTA		N							
ATOM	70	CA	LEU		67	34.134	35.206	28.529	1.00 17.36
MOTA	71	С	LEU	Α	67	35.295	34.328	28.985	1.00 16.04
MOTA	72	0	LEU	Α	67	36.499	34.701	28.842	1.00 16.38
ATOM	73	CB	LEU	A	67	33.707	34.757	27.128	1.00 17.19
MOTA	74	CG	LEU	Α	67	32.226	34.504	26.839	1.00 18.63
ATOM	75		LEU		67	31.349	35.604	27.407	1.00 16.94
	76		LEU		67	32.049	34.375	25.330	1.00 18.67
MOTA							33.166	29.531	1.00 14.58
MOTA	77	N	ARG		68	34.956			
ATOM	78	CA	ARG		68	35.961	32.173	29.973	1.00 16.73
MOTA	79	С	ARG	Α	68	35.394	30.775	29.717	1.00 15.78
MOTA	80	0	ARG	Α	68	34.154	30.610	29.500	1.00 13.85
ATOM	81	CB	ARG	Α	68	36.299	32.349	31.459	1.00 18.19
ATOM	82	CG	ARG		68	37.086	33.623	31.766	1.00 21.67
ATOM	83	CD	ARG		68	37.571	33.646	33.213	1.00 23.25
					68	36.462	33.653	34.165	1.00 26.34
MOTA	84	NE	ARG						
ATOM	85	CZ	ARG		68	36.598	33.500	35.482	1.00 27.29
MOTA	86		ARG		68	37.802	33.324	36.015,	
MOTA	87	NH2	ARG	Α	68	35.530	33.527	36.271	1.00 26.77
ATOM	88	N	GLY	Α	69	36.262	29.769	29.726	1.00 14.89
ATOM	89	CA	GLY	Α	69	35.816	28.409	29.486	1.00 15.62
ATOM	90	С	GLY		69	36.505	27.806	28.277	1.00 16.66
ATOM	91	ō	GLY		69	37.526	28.367	27.771	1.00 15.60
								27.804	1.00 17.25
ATOM	92	N	LYS		70	35.989	26.676		
MOTA	93	CA	LYS		70	36.556	25.973	26.629	1.00 16.95
MOTA	94	С	LYS	Α	70	35.472	25.138	25.949	1.00 16.87
MOTA	95	0	LYS	Α	70	34.394 [,]	24.864	26.562	1.00 17.19
ATOM	96	CB	LYS	Α	70	37.737	25.092	27.058	1.00 18.62
ATOM	97	CG	LYS	A	70	37.518	24.303	28.348	1.00 19.97
ATOM	98	CD	LYS		70	38.737	23.446	28.667	1.00 22.43
ATOM	99	CE	LYS		70	38.538	22.611	29.926	1.00 23.77
					70	39.660	21.638	30.129	1.00 22.43
ATOM	100	NZ	LYS						
MOTA	101	N	SER		71	35.714	24.729	24.706	1.00 15.11
MOTA	102	CA	SER		71	34.706	23.950	23.940	1.00 14.34
MOTA	103	С	SER	Α	71	34.155	22.730	24.667	1.00 14.36
MOTA	104	0	SER	Α	71	32.918	22.446	24.600	1.00 13.81
MOTA	105	CB	SER	Α	71	35.281	23.523	22.581	1.00 14.97
ATOM	106	OG	SER		71	36.456	22.743	22.732	1.00 15.41
ATOM	107	N	GLY		72	35.024	22.005	25.362	1.00 14.38
	108	CA	GLY		72	34.588	20.815	26.072	1.00 14.63
MOTA									1.00 16.49
ATOM	109	C	GLY		72	33.661	21.022	27.262	
MOTA	110	0	GLY		72	32.772	20.159	27.537	1.00 16.20
MOTA	111	N	GLN	Α	73	33.814	22.129	27.979	1.00 16.78
MOTA	112	CA	GLN	Α	73	32.965	22.369	29.167	1.00 18.67
MOTA	113	С	GLN	Α	73	32.040	23.570	29.038	1.00 18.70
ATOM	114	0.	GLN		73	31.223	23.858	29.967	1.00 19.81
ATOM	115	CB	GLN		73	33.852	22.522	30.401	1.00 20.09
	116	CG			73 73	34.924	21.433	30.493	1.00 24.21
ATOM			GLN						
ATOM	117	CD	GLN		73	35.624	21.400	31.837	1.00 24.83
MOTA	118	OE1			73	36.048	22.467	32.380	1.00 26.53
MOTA	119	NE2	GLN		73	35.769	20.206	32.395	1.00 25.73
MOTA	120	N	GLY	Α	74	32.138	24.274	27.914	1.00 17.65

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ATOM	121	CA	GLY		74	31.292	25.429	27.688	1.00 15.83
MOTA	122	С	GLY	Α	74	31.939	26.746	28.068	1.00 15.56
MOTA	123	0	GLY	Α	74	32.837	26.799	28.962	1.00 17.53
ATOM	124	N	TYR	Α	75	31.517	27.814	27.403	1.00 13.96
MOTA	125	CA	TYR		75	32.041	29.164	27.686	1.00 16.12
ATOM	126	С	TYR		75	30.991	29.903	28.502	1.00 14.92
MOTA	127	0	TYR	Α	75	29.758	29.793	28.217	1.00 14.71
ATOM	128	CB	TYR	Α	75	32.324	29.918	26.385	1.00 17.79
MOTA	129	CG	TYR	Α	75	33.490	29.354	25.605	1.00 18.92
ATOM	130	CD1			75	33.326	28.271	24.742	1.00 19.83
MOTA	131	CD2	TYR		75	34.763	29.909	25.735	1.00 20.43
MOTA	132	CE1	TYR		75	34.409	27.757	24.020	1.00 21.98
MOTA	133	CE2	TYR	Α	75	35.847	29.407	25.025	1.00 21.04
MOTA	134	CZ	TYR	Α	75	35.666	28.339	24.170	1.00 22.04
ATOM	135	ОН	TYR		75	36.746	27.882	23.456	1.00 22.86
	136	N	TYR		76	31.432	30.653	29.507	1.00 13.66
MOTA									
ATOM	137	CA	TYR		76	30.478	31.360	30.368	1.00 12.95
MOTA	138	С	TYR	A	76	30.753	32.837	30.593	1.00 13.47
MOTA	139	0	TYR	A	76	31.901	33.345	30.391	1.00 13.77
ATOM	140	CB	TYR	Α	76	30.395	30.662	31.725	1.00 13.31
ATOM	141	CG	TYR	Α	76	31.723	30.548	32.446	1.00 14.55
ATOM	142	CD1			76	32.601	29.497	32.174	1.00 16.16
MOTA	143	CD2	TYR		76	32.105	31.495	33.392	1.00 15.68
MOTA	144	CE1	TYR	Α	76	33.829	29.392	32.832	1.00 17.64
MOTA	145	CE2	TYR	Α	76	33.329	31.402	34.055	1.00 18.14
ATOM	146	CZ	TYR	A	76	34.183	30.348	33.770	1.00 18.24
ATOM	147	OH	TYR	Α	76	35.390	30.252	34.428	1.00 21.79
ATOM	148	N	VAL		77	29.716	33.546	31.017	1.00 12.55
	149	CA	VAL		77	29.844	34.980	31.298	1.00 14.17
ATOM									
MOTA	150	C	VAL		77	29.390	35.225	32.727	1.00 15.16
MOTA	151	0	VAL		77	28.564	34.439	33.283	1.00 16.09
MOTA	152	CB	VAL	Α	77	28.975	35.821	30.336	1.00 13.43
MOTA	153	CG1	VAL	A	77	27.495	35.528	30.567	1.00 11.59
MOTA	154	CG2	VAL	Α	77	29.281	37.305	30.524	1.00 10.74
ATOM	155	N	GLU		78	29.905	36.276	33.352	1.00 16.88
	156	CA	GLU		78	29.486	36.571	34.731	1.00 17.45
ATOM									
MOTA	157	C	GLU		78	28.178	37.345	34.706	1.00 16.89
ATOM	158	0	GLU		78	27.961	38.239	33.826	1.00 14.65
MOTA	159	CB	GLU	Α	78	30.538	37.392	35.479	1.00 19.11
MOTA	160	CG	GLU	Α	78	30.222	37.503	36.974	1.00 24.70
MOTA	161	CD	GLU	Α	78	31.225	38.342	37.757	1.00 26.24
MOTA	162	OE1			78	31.162	39.584	37.679	1.00 27.53
ATOM	163	OE2	GLU		78	32.076	37.755	38.452	1.00 29.49
	164	N	MET		70 79	27.296	37.733	35.641	1.00 25.45
ATOM									
ATOM	165	CA	MET		79	25.992	37.684	35.761	1.00 17.22
MOTA	166	C	MET		79	25.610	37.768	37.232	1.00 17.77
MOTA	167	0	MET	Α	79	26.208	37.066	38.100	1.00 18.29
ATOM	168	CB	MET	Α	79	24.908	36.899	35.007	1.00 16.88
ATOM	169	CG	MET		79	25.070	36.874	33.492	1.00 16.65
ATOM	170	SD	MET		79	23.798	35.865	32.673	1.00 17.43
MOTA	171	CE	MET		79	22.442	37.003	32.577	1.00 15.55
ATOM	172	И	THR		80	24.637	38.617	37.539	1.00 17.73
MOTA	173	CA	THR	A	80	24.146	38.741	38.917	1.00 17.50
ATOM	174	С	THR	A	80	22.632	38.630	38.853	1.00 17.85
MOTA	175	0	THR	A	80	21.995	39.075	37.851	1.00 17.14
ATOM	176	СВ	THR		80	24.524	40.100	39.550	1.00 18.12
ATOM	177	OG1			80	23.851	41.158	38.857	1.00 18.55
ATOM	178	CG2	THR		80	26.031	40.328	39.474	1.00 16.48
MOTA	179	N	VAL		81	22.042	38.020	39.874	1.00 18.24
ATOM	180	CA	VAL		81	20.573	37.882	39.959	1.00 20.23
MOTA	181	С	VAL	A	81	20.145	38.274	41.375	1.00 21.18
ATOM	182	0	VAL	Α	81	20.929	38.093	42.362	1.00 20.31

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MOTA	183	CB	VAL	Α	81	20.105	36.429	39.700	1.00 20.43
ATOM	184	CG1	VAL	A	81	20.566	35.959	38.334	1.00 21.49
MOTA	185		VAL		81	20.639	35.518	40.777	1.00 21.78
MOTA	186	N	GLY		82	18.938	38.817	41.497	1.00 21.84
MOTA	187	CA	·GLY	Α	82	18.421	39.200	42.799	1.00 21.10
MOTA	188	С	GLY	Α	82	18.973	40.475	43.404	1.00 21.47
ATOM	189	Ö	GLY		82	19.864	41.159	42.814	1.00 21.97
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MOTA	190	N	SER		83	18.454	40.808	44.581	1.00 22.27
ATOM	191	CA	SER	Α	83	18.869	42.012	45.335	1.00 22.02
ATOM	192	С	SER	Α	83	18.996	41.607	46.795	1.00 20.16
MOTA	193	Ō	SER		83	18.002	41.120	47.410	1.00 20.07
ATOM	194	CB	SER		83	17.804	43.104	45.213	1.00 21.98
MOTA	195	OG	SER	Α	83	17.356	43.229	43.874	1.00 23.70
MOTA	196	N	PRO	Α	84	20.198	41.734	47.380	1.00 21.14
ATOM	197	CA	PRO	Α	84	21.454	42.221	46.785	1.00 20.45
ATOM	198	C	PRO		84	21.911	41.288	45.656	1.00 20.37
MOTA	199	0	PRO		84	21.508	40.086	45.606	1.00 18.46
MOTA	200	CB	PRO	A	84	22.434	42.193	47.962	1.00 19.74
ATOM	201	CG	PRO	Α	84	21.548	42.320	49.166	1.00 20.71
MOTA	202	CD	PRO	Α	84	20.377	41.447	48.815	1.00 19.44
ATOM	203	N	PRO		85	22.754	41.790	44.741	1.00 20.53
MOTA	204	CA	PRO		85	23.258	40.997	43.616	1.00 20.58
MOTA	205	С	PRO	Α	85	23.949	39.706	44.046	1.00 20.81
MOTA	206	0	PRO	Α	85	24.854	39.720	44.936	1.00 21.15
MOTA	207	СВ	PRO	Α	85	24.240	41.947	42.932	1.00 20.87
ATOM	208	CG	PRO		85	23.732	43.294	43.282	1.00 22.23
MOTA	209	CD	PRO		85	23.340	43.141	44.724	1.00 21.41
MOTA	210	N	GLN	Α	86	23.541	38.590	43.453	1.00 20.05
ATOM	211	CA	GLN	Α	86	24.174	37.289	43.752	1.00 19.63
ATOM	212	C	GLN		86	24.904	36.923	42.472	1.00 20.50
ATOM	213	ō	GLN		86				
						24.263	36.622	41.412	1.00 19.85
MOTA	214	СВ	GLN		86	23.127	36.227	44.097	1.00 19.82
MOTA	215	CG	\mathtt{GLN}	Α	86	22.283	36.586	45.314	1.00 18.97
MOTA	216	CD	GLN	Α	86	21.292	35.506	45.693	1.00 19.84
ATOM	217	OE1			86	20.226	35.801	46.316	1.00 21.21
ATOM	218	NE2	GLN		86				
						21.603	34.259	45.354	1.00 17.54
ATOM	219	N	THR		87	26.229	36.969	42.527	1.00 19.61
MOTA	220	CA	THR	Α	87	27.057	36.669	41.346	1.00 19.61
ATOM	221	С	THR	Α	87	27.088	35.188	40.994	1.00 18.63
ATOM	222	0	THR		87	27.220	34.302	41.892	1.00 18.56
ATOM	223	СВ	THR		87	28.501			
							37.164	41.549	•
MOTA	224	OG1			87	28.486	38.558	41.887	1.00 20.57
MOTA	225	CG2	THR	Α	87	29.304	36.977	40.278	1.00 18.65
ATOM	226	N	LEU	A	88	26.972	34.907	39.701	1.00 18.38
ATOM	227	CA	LEU	Α	88	26.991	33.522	39.193	1.00 18.18
ATOM	228	C	LEU		88	27.572	33.496	37.781	1.00 18.11
	229								
ATOM		0	LEU		88	27.353	34.457	36.974	1.00 18.86
ATOM	230	CB	LEU	A	88	25.568	32.952	39.159	1.00 16.21
MOTA	231	CG	LEU	Α	88	24.825	32.828	40.495	1.00 18.20
MOTA	232	CD1	LEU		88	23.366	32.474	40.226	1.00 18.10
ATOM	233		LEU		88	25.484	31.766		
								41.379	
MOTA	234	N	ASN		89	28.317	32.443	37.459	1.00 15.84
MOTA	235	CA	ASN	A	89	28.876	32.312	36.101	1.00 16.22
MOTA	236	С	ASN	Α	89	27.841	31.544	35.300	1.00 16.03
ATOM	237	0	ASN		89	27.363	30.450	35.735	1.00 15.05
ATOM	238	СВ	ASN		89				
						30.208	31.565	36.114	1.00 15.71
MOTA	239	CG	ASN		89	31.324	32.396	36.700	1.00 16.10
MOTA	240		ASN		89	31.390	33.650	36.477	1.00 15.48
MOTA	241	ND2	ASN	Α	89	32.217	31.750	37.439	1.00 14.07
ATOM	242	N	ILE	A	90	27.485	32.091	34.145	1.00 15.55
ATOM	243	CA	ILE		90	26.445	31.494	33.292	1.00 14.59
ATOM	244	C							
WI OLI	644	C	ILE	W	90	26.960	31.052	31.930	1.00 15.07

ATOM	245	0	ILE	Α	90	27.578	31.867	31.173	1.00 13.01
ATOM	246	СВ	ILE		90	25.301	32.512	33.084	1.00 14.44
ATOM	247	CG1	ILE		90	24.884	33.098	34.437	1.00 14.15
ATOM	248	CG2	ILE		90	24.114	31.847	32.407	1.00 14.29
	249	CD1	ILE		90	24.356	32.062	35.426	1.00 13.44
MOTA					91	26.714	29.790	31.590	1.00 15.08
ATOM	250	N	LEU						
ATOM	251	CA	LEU		91	27.153	29.249	30.284	1.00 15.63
MOTA	252	С	LEU		91	26.313	29.878	29.174	1.00 16.04
ATOM	253	0	LEU		91	25.041	29.904	29.250	1.00 16.72
MOTA	254	CB	LEU		91	27.008	27.721	30.265	1.00 14.67
ATOM	255	CG	PEA	Α	91	27.450	26.945	29.012	1.00 15.49
ATOM	256	CD1	LEU	A	91	27.692	25.485	29.364	1.00 15.10
ATOM	257	CD2	LEU	A	91	26.393	27.052	27.925	1.00 15.54
ATOM	258	N	VAL	Α	92	26.995	30.408	28.164	1.00 16.13
ATOM	259	CA	VAL	A	92	26.336	31.051	27.003	1.00 15.39
ATOM	260	С	VAL	Α	92	25.901	29.960	26.038	1.00 15.51
ATOM	261	ō	VAL		92	26.761	29.243	25.440	1.00 16.92
MOTA	262	СВ	VAL		92	27.306	32.008	26.278	1.00 15.40
ATOM	263	CG1			92	26.668	32.523	24.994	1.00 16.99
ATOM	264	CG2	VAL		92	27.671	33.172	27.200	1.00 13.64
MOTA	265	N	ASP		93	24.594	29.824	25.845	1.00 16.41
	266		ASP		93	24.069	28.762	24.974	1.00 10.41
MOTA		CA							
MOTA	267	C	ASP		93	23.090	29.226	23.903	1.00 15.40
ATOM	268	0	ASP		93	21.889	29.494	24.206	1.00 15.81
MOTA	269	CB	ASP		93	23.411	27.701	25.861	1.00 16.00
MOTA	270	CG	ASP		93	22.897	26.512	25.078	1.00 16.45
MOTA	271	OD1	ASP		93	23.536	26.133	24.076	1.00 17.23
MOTA	272	OD2	ASP		93	21.863	25.938	25.481	1.00 16.68
MOTA	273	N	THR	A	94	23.550	29.326	22.657	1.00 13.38
MOTA	274	CA	THR	A	94	22.636	29.745	21.574	1.00 13.70
ATOM	275	С	THR	Α	94	21.811	28.549	21.109	1.00 13.68
MOTA	276	0	THR	Α	94	20.941	.28.671	20.190	1.00 14.18
ATOM	277	CB	THR	Α	94	23.397	30.349	20.362	1.00 14.99
ATOM	278	OG1	THR	Α	94	24.279	29.370	19.798	1.00 14.96
ATOM	279	CG2	THR		94	24.201	31.568	20.794	1.00 14.04
ATOM	280	N	GLY		95	22.053	27.392	21.719	1.00 14.90
ATOM	281	CA	GLY		95	21.309	26.199	21.351	1.00 15.51
ATOM	282	C	GLY		95	20.108	25.969	22.255	1.00 16.96
ATOM	283	Ö	GLY		95	19.516	24.850	22.275	1.00 16.90
ATOM	284	N	SER		96	19.721	26.987	23.011	1.00 17.38
ATOM	285	CA	SER		96	18.562	26.851	23.922	1.00 17.35
ATOM	286	C	SER		96	17.990	28.231	24.226	1.00 17.07
	287	o							1.00 17.07
ATOM	288	СВ	SER		96 96	18.573	29.269	23.803	1.00 14.54
ATOM			SER			19.005	26.174	25.219	
ATOM	289	OG	SER		96	19.640	26.894	26.276	1.00 26.99
ATOM	290	N	SER		97	16.869	28.292	24.936	1.00 16.25
ATOM	291	CA	SER		97	16.290	29.614	25.258	1.00 18.39
MOTA	292	C	SER		97	15.740	29.776	26.670	1.00 17.83
ATOM	293	0	SER		97	14.866	30.653	26.932	1.00 18.75
ATOM	294	CB	SER		97	15.224	29.993	24.227	1.00 18.88
ATOM	295	OG	SER		97	14.633	28.850	23.651	1.00 23.68
MOTA	296	N	ASN	Α	98	16.229	28.959	27.592	1.00 17.57
MOTA	297	CA	ASN		98	15.809	29.073	28.993	1.00 16.01
MOTA	298	C	ASN	A	98	16.963	29.611	29.821	1.00 16.51
ATOM	299	0	ASN	Α	98	18.127	29.109	29.709	1.00 16.69
ATOM	300	СВ	ASN		98	15.401	27.720	29.566	1.00 13.74
ATOM	301	CG	ASN		98	13.969	27.359	29.241	1.00 16.04
ATOM	302		ASN		98	13.669	26.795	28.139	1.00 13.27
ATOM	303	ND2	ASN		98	13.058	27.680	30.158	1.00 13.26
ATOM	304	N	PHE		99	16.688	30.640	30.614	1.00 14.45
ATOM	305	CA	PHE		99	17.710	31.196	31.519	1.00 13.19
ATOM	306	C	PHE		99	17.453	30.424	32.812	1.00 13.23
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MOTA	307	0	PHE A		16.319	30.466	33.384	1.00 11.00
ATOM	308	CB	PHE A		17.491	32.699	31.722	1.00 13.54
MOTA	309	CG	PHE A		18.390	33.318	32.761	1.00 14.79
MOTA	310	CD1			19.741	32.978	32.836	1.00 15.02
MOTA	311	CD2	PHE A		17.889	34.258	33.657	1.00 16.17
MOTA	312	CE1	PHE A		20.576	33.564	33.784	1.00 14.99
ATOM	313	CE2	PHE A		18.718	34.852	34.610	1.00 16.36
ATOM	314	CZ	PHE A		20.064	34.503	34.674	1.00 14.33
ATOM	315	N	ALA A		18.457	29.691	33.274 34.497	1.00 11.83 1.00 12.34
ATOM	316	CA	ALA A		18.298 19.594	28.889 28.836	35.277	1.00 12.34
ATOM ATOM	317 318	С 0	ALA A		20.722	28.896	34.684	1.00 14.33
ATOM	319	СВ	ALA A		17.849	27.486	34.138	1.00 13.19
ATOM	320	N	VAL A		19.467	28.727	36.595	1.00 13.51
ATOM	321	CA	VAL A		20.640	28.686	37.473	1.00 13.80
ATOM	322	C	VAL A		20.429	27.693	38.610	1.00 15.86
ATOM	323	ō	VAL A		19.253	27.424	39.031	1.00 13.90
ATOM	324	СВ	VAL A		20.912	30.082	38.075	1.00 14.68
ATOM	325		VAL A		21.126	31.098	36.962	1.00 12.49
ATOM	326	CG2	VAL A		19.743	30.509	38.953	1.00 13.11
MOTA	327	N	GLY A	102	21.528	27.120	39.098	1.00 16.51
MOTA	328	CA	GLY A	102	21.437	26.189	40.207	1.00 17.46
MOTA	329	C	GLY A	102	20.858	26.966	41.375	1.00 19.61
MOTA	330	0	GLY A		21.303	28.128	41.641	1.00 19.12
MOTA	331	N	ALA A		19.875	26.395	42.065	1.00 19.81
ATOM	332	CA	ALA A		19.241	27.092	43.212	1.00 22.41
ATOM	333	С	ALA A		19.098	26.169	44.414	1.00 23.71
ATOM	334	0	ALA A		18.196	26.366	45.293	1.00 24.50
ATOM	335	CB	ALA A		17.880	27.627	42.807	1.00 21.12
ATOM	336	N	ALA A		19.967	25.168	44.470	1.00 23.53
ATOM	337	CA	ALA A		19.979	24.180	45.566	1.00 24.47
ATOM	338	C	ALA A		21.341	23.505	45.517	1.00 24.98
ATOM	339	0	ALA A		21.974	23.413	44.419	1.00 26.65 1.00 23.55
ATOM ATOM	340 341	CB N	ALA A PRO A		18.869 21.836	23.150 23.026	45.367 46.668	1.00 25.27
ATOM	342	CA	PRO A		23.140	22.361	46.733	1.00 23.27
ATOM	343	C	PRO A		23.328	21.286	45.672	1.00 24.16
ATOM	344	ō	PRO A		22.350	20.594	45.251	1.00 24.35
ATOM	345	СВ	PRO A		23.159	21.778	48.143	1.00 25.36
ATOM	346	ÇG	PRO A		22.347	22.763	48.920	1.00 25.71
ATOM	347	CD	PRO A		21.183	23.020	47.990	1.00 25.99
ATOM	348	N	HIS A	106	24.566	21.135	45.227	1.00 24.93
MOTA	349	CA	HIS A	106	24.918	20.119	44.223	1.00 23.63
MOTA	350	C	HIS A	106	26.402	19.843	44.367	1.00 24.29
MOTA	351	0	HIS A	106	27.207	20.790	44.596	1.00 24.19
ATOM	352	СВ	HIS A	106	24.646	20.622	42.807	1.00 24.15
ATOM	353	CG	HIS A		24.887	19.587	41.756	1.00 24.43
ATOM	354		HIS A		23.912	18.702	41.348	1.00 25.53
MOTA	355		HIS A		26.012	19.244	41.084	1.00 23.79
ATOM	356		HIS A		24.426	17.857	40.471	1.00 25.66
ATOM	357		HIS A		25.699	18.164	40.294	1.00 24.92
ATOM	358	N	PRO A		26.811	18.572	44.236	1.00 25.36
MOTA	359	CA	PRO A		28.224	18.200	44.358	1.00 26.23
ATOM	360	C	PRO A		29.164	19.025	43.474	1.00 26.26
ATOM ATOM	361	O	PRO A		30.335	19.296	43.866	1.00 28.01 1.00 26.21
ATOM	362 363	CB			28.225 26.875	16.722	43.972	
ATOM	364	CG CD	PRO A		25.977	16.259 17.384	44.418. 43.971	1.00 25.73
ATOM	365	N	PHE A		28.695	17.384	43.971	1.00 25.04
MOTA	366	CA	PHE A		29.556	20.218	42.299	1.00 26.76
ATOM	367	C	PHE A		29.358	21.726	41.450	1.00 26.66
ATOM	368	0	PHE A		30.103	22.494	40.778	1.00 26.81
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MOTA	369	CB	PHE	A	108	29.368	19.754	39.936	1.00 26.67
ATOM	370	CG	PHE	Δ	108	29.665	18.300	39.720	1.00 26.80
						30.531	17.614	40.569	1.00 27.67
MOTA	371		PHE						
MOTA	372	CD2	PHE	Α	108	29.090	17.615	38.655	1.00 27.12
ATOM	373	CE1	PHE	Α	108	30.819	16.262	40.359	1.00 27.99
ATOM	374	CE2	PHE			29.369	16.267	38.433	1.00 26.65
			PHE			30.235	15.587	39.286	1.00 26.94
MOTA	375	CZ							
MOTA	376	N	LEU			28.386	22.180	42.231	1.00 26.14
MOTA	377	CA	LEU	Α	109	28.144	23.629	42.346	1.00 27.17
ATOM	378	С	LEU	Α	109	28.914	24.248	43.510	1.00 29.20
ATOM	379	ō	LEU			28.861	23.743	44.669	1.00 26.91
						26.647		42.498	1.00 25.73
ATOM	380	CB	LEU				23.911		
MOTA	381	CG	LEU			25.811	23.714	41.230	1.00 25.94
ATOM	382	CD1	LEU	Α	109	24.343	23.983	41.530	1.00 24.99
ATOM	383	CD2	LEU	Α	109	26.310	24.657	40.136	1.00 24.26
ATOM	384	N	HIS			29.632	25.328	43.213	1.00 32.94
						30.442	26.077	44.207	1.00 35.82
ATOM	385	CA	HIS						
ATOM	386	С	HIS			29.533	27.015	44.983	1.00 33.93
ATOM	387	0	HIS	Α	110	29.732	27.265	46.209	1.00 34.20
MOTA	388	CB	HIS	А	110	31.501	26.915	43.485	1.00 42.49
ATOM	389	CG	HIS			32.907	26.469	43.732	1.00 47.84
			HIS			33.509	26.558	44.969	1.00 50.74
ATOM	390								
ATOM	391		HIS			33.834	25.934	42.899	1.00 49.74
ATOM	392	CE1	${ t HIS}$	Α	110	34.746	26.098	44.888	1.00 51.83
ATOM	393	NE2	HIS	Α	110	34.968	25.713	43.644	1.00 51.38
ATOM	394	N	ARG			28.547	27.553	44.279	1.00 31.13
			ARG			27.579	28.494	44.857	1.00 28.72
ATOM	395	CA							
ATOM	396	С	ARG			26.287	28.331	44.072	1.00 28.16
ATOM	397	0	ARG	Α	111	26.267	27.652	43.000	1.00 27.40
ATOM	398	СВ	ARG	Α	111	28.108	29.924	44.717	1.00 28.09
ATOM	399	CG	ARG			28.550	30.255	43.305	1.00 26.48
						29.216	31.616	43.201	1.00 25.86
ATOM	400	CD	ARG						
MOTA	401	NE	ARG	Α	111	29.723	31.831	41.849	1.00 25.21
ATOM	402	CZ	ARG	Α	111	30.423	32.892	41.465	1.00 24.44
MOTA	403	NH1	ARG	Α	111	30.708	33.850	42.337	1.00 25.08
ATOM	404	NH2	ARG			30.828	32.995	40.205	1.00 22.62
ATOM	405	N	TYR			25.207	28.922	44.566	1.00 26.27
ATOM	406	CA	TYR			23.922	28.814	43.866	1.00 23.70
MOTA	407	С	TYR	Α	112	22.955	29.916	44.250	1.00 22.77
ATOM	408	0	TYR .	Α	112	23.140	30.633	45.283	1.00 21.10
ATOM	409	CB	TYR .	Α	112	23.295	27.437	44.119	1.00 25.47
ATOM	410	CG	TYR			23.036	27.111	45.575	1.00 27.20
ATOM	411		TYR			21.885		46.222	1.00 28.51
							27.569		
MOTA	412		TYR			23.946	26.353	46.309	1.00 27.51
ATOM	413	CE1	TYR .	Α	112	21.647	27.276	47.565	1.00 27.78
MOTA	414	CE2	TYR .	Α	112	23.720	26.058	47.651	1.00 28.63
ATOM	415	CZ	TYR .			22.570	26.522	48.270	1.00 28.98
ATOM	416	OH	TYR			22.352	26.228	49.591	1.00 30.28
ATOM	417	N	TYR			21.927	30.069	43.428	1.00 19.32
ATOM	418	CA	TYR .	A	113	20.896	31.090	43.624	1.00 18.94
ATOM	419	С	TYR	Α	113	20.047	30.807	44.857	1.00 17.90
ATOM	420	0	TYR .	A	113	19.480	29.688	45.011	1.00 19.37
ATOM	421	СВ				20.027		42.369	1.00 17.76
			TYR .				31.141		
ATOM	422	CG	TYR .			18.887	32.135	42.378	1.00 17.68
ATOM	423		TYR			19.024	33.397	42.963	1.00 16.86
MOTA	424	CD2	TYR .	Α	113	17.709	31.854	41.688	1.00 16.79
ATOM	425	CE1	TYR .	Α	113	18.020	34.349	42.848	1.00 17.05
ATOM	426		TYR .			16.704	32.796	41.563	1.00 16.02
									1.00 17.36
MOTA	427	CZ	TYR .			16.858	34.038	42.138	
MOTA	428	OH	TYR .			15.848	34.963	41.984	1.00 16.62
MOTA	429	N	GLN .	A	114	19.967	31.790	45.746	1.00 18.68
MOTA	430	CA	GLN .	Α	114	19.156	31.673	46.983	1.00 20.28

MOTA	431	С	GLN	Α	114	18.057	32.719	46.897	1.00 19.59
MOTA	432	0	GLN	Α	114	18.285	33.933	47.192	1.00 20.34
ATOM	433	СВ	GLN	Α	114	20.028	31.912	48.216	1.00 19.79
MOTA	434	CG	GLN	A	114	21.048	30.814	48.434	1.00 22.79
MOTA	435	CD	GLN	Α	114	21.942	31.063	49.626	1.00 24.34
ATOM	436	OE1	GLN	Α	114	22.708	32.073	49.668	1.00 26.47
ATOM	437	NE2			114	21.876	30.173	50.606	1.00 24.49
MOTA	438	N			115	16.876	32.275	46.479	1.00 20.48
ATOM	439	CA			115	15.703	33.159	46.305	1.00 21.24
MOTA	440	C			115	15.234	33.837	47.583	1.00 21.94
ATOM	441	ō			115	14.784	35.022	47.546	1.00 21.40
MOTA	442	СВ			115	14.550	32.366	45.686	1.00 20.21
ATOM	443	CG			115	14.807	31.953	44.240	1.00 20.21
ATOM	444	CD			115	13.917	30.796	43.824	1.00 20.32
ATOM	445	NE			115	14.305	29.567	44.508	1.00 20.45
ATOM	446	CZ			115	13.626	28.428	44.448	1.00 20.43
ATOM	447	NH1			115	12.514	28.352	43.732	1.00 20.02
ATOM	448					14.061	27.366	45.106	1.00 20.02
ATOM	449	N			116	15.323	33.138	48.710	1.00 22.93
ATOM	450	CA			116	14.880	33.723	49.993	1.00 24.99
ATOM	451	C			116	15.718	34.953	50.343	1.00 23.86
	452	0			116	15.242	35.873	51.080	1.00 24.27
MOTA MOTA	453	СВ			116	14.972	32.691	51.123	1.00 24.27
ATOM	454	CG			116	16.391	32.280	51.502	1.00 27.81
ATOM	455	CD			116	16.999	31.257	50.550	1.00 36.05
ATOM	456	OE1				16.955	31.423	49.295	1.00 36.88
	457	NE2	GLN			17.577	30.199	51.112	1.00 37.21
ATOM ATOM	458	NEZ N			117	16.944	35.006	49.833	1.00 37.21
	459	CA	LEU			17.831	36.153	50.112	1.00 20.59
ATOM								49.124	
ATOM	460	С	LEU			17.673 18.440	37.296	49.124	1.00 19.96 1.00 18.93
ATOM	461	0			117	19.296	38.301	50.128	
ATOM	462	CB	LEU				35.707		1.00 21.68 1.00 22.49
ATOM	463	CG	LEU			19.887	35.224	51.454	1.00 22.49
ATOM	464		LEU			19.001 21.286	34.175	52.074	1.00 22.03
ATOM	465		LEU				34.675	51.210	
ATOM	466	N			118	16.714	37.183	48.210	1.00 18.14
ATOM	467	CA			118	16.484	38.252	47.208	1.00 17.08
ATOM	468	C	SER			15.150	38.953	47.436	1.00 16.25
MOTA	469	0	SER			14.055	38.316	47.347	1.00 16.00
ATOM	470	CB	SER			16.519	37.679	45.787	1.00 15.12
MOTA	471	OG	SER			16.301	38.708	44.835	1.00 16.81
MOTA	472	N	SER			15.210	40.250	47.711	1.00 15.31
MOTA	473	CA	SER			13.991	41.044	47.973	1.00 18.09
ATOM	474	C	SER				41.307	46.714 46.800	1.00 17.35 1.00 17.62
ATOM ATOM	475 476	0	SER			11.964 14.371	41.669	48.618	1.00 17.82
ATOM	477	CB	SER				42.380		1.00 18.71
		OG	SER			15.158	43.160	47.727	
MOTA	478	N	THR			13.781	41.137	45.546	1.00 18.90
MOTA	479	CA	THR			13.075	41.381	44.263	1.00 17.26
MOTA	480	C	THR			12.587	40.104	43.594	1.00 17.17
MOTA	481	0	THR			12.004	40.139	42.466	1.00 18.70
ATOM	482	CB	THR			13.980	42.143	43.283	1.00 17.78
MOTA	483	OG1				15.305	41.609	43.355	1.00 17.35
MOTA	484	CG2				14.012	43.630	43.624	1.00 17.37
MOTA	485	N	TYR			12.800	38.977	44.257	1.00 18.03
MOTA	486	CA	TYR			12.364	37.676	43.715	1.00 18.53
MOTA	487	C	TYR			10.841	37.584	43.606	1.00 18.12
MOTA	488	0	TYR			10.088	38.028	44.531	1.00 19.29
MOTA	489	CB	TYR			12.878	36.547	44.607	1.00 18.32
MOTA	490	CG	TYR			12.187	35.225	44.368	1.00 22.03
MOTA	491	CD1				12.429	34.484	43.209	1.00 21.48
MOTA	492	CD2	TYR	A	121	11.268	34.725	45.291	1.00 21.95

MOTA	493	CE1	TYR	Α	121	11.776	33.280	42.977	1.00 21.33
MOTA	494	CE2	TYR	Α	121	10.608	33.523	45.067	1.00 22.77
MOTA	495	CZ	TYR	A	121	10.867	32.807	43.908	1.00 23.35
ATOM	496	ОН	TYR	A	121	10.206	31.622	43.682	1.00 23.63
ATOM	497	N			122	10.365	37.039	42.492	1.00 16.86
ATOM	498	CA			122	8.909	36.851	42.281	1.00 16.79
ATOM	499	C			122	8.703	35.397	41.890	1.00 17.46
ATOM	500	Ö			122	9.348	34.884	40.924	1.00 17.88
		-							
ATOM	501	CB			122	8.384	37.764	41.174	1.00 14.87
ATOM	502	CG			122	8.335	39.230	41.548	1.00 14.83
ATOM	503	CD			122	7.895	40.067	40.369	1.00 14.98
MOTA	504	NE			122	7.822	41.481	40.706	1.00 16.19
ATOM	505	\mathbf{cz}			122	7.546	42.442	39.833	1.00 16.67
MOTA	506		ARG			7.316	42.142	38.559	1.00 15.67
MOTA	507	NH2	ARG			7.505	43.704	40.233	1.00 16.38
ATOM	508	N	ASP	Α	123	7.836	34.720	42.628	1.00 18.52
ATOM	509	CA	ASP	Α	123	7.538	33.296	42.388	1.00 19.00
ATOM	510	С	ASP	Α	123	6.435	33.147	41.347	1.00 19.87
ATOM	511	0	ASP	A	123	5.342	33.757	41.490	1.00 17.59
MOTA	512	СВ	ASP	Α	123	7.090	32.657	43.702	1.00 19.80
ATOM	513	CG	ASP			6.841	31.171	43.582	1.00 20.76
ATOM	514		ASP			6.933	30.615	42.463	1.00 20.41
ATOM	515		ASP			6.549	30.559	44.629	1.00 22.50
ATOM	516	N	LEU			6.689	32.359	40.305	1.00 20.70
ATOM	517	CA	LEU			5.672	32.139	39.255	1.00 21.20
			LEU			4.790		39.562	1.00 21.20
ATOM	518	C					30.929		
ATOM	519	0	LEU			3.832	30.601	38.786	1.00 21.17
ATOM	520	CB	LEU			6.343	31.978	37.888	1.00 21.51
ATOM	521	CG	LEU			6.850	33.288	37.270	1.00 22.05
ATOM	522		LEU			7.617	32.994	35.997	1.00 22.23
MOTA	523		LEU			5.678	34.217	36.983	1.00 21.49
MOTA	524	N	ARG			5.083	30.252	40.666	1.00 22.67
MOTA	525	CA	ARG	Α	125	4.286	29.078	41.085	1.00 25.58
MOTA	526	С	ARG	Α	125	4.106	28.081	39.944	1.00 26.39
MOTA	527	0	ARG	Α	125	2.974	27.552	39.719	1.00 26.83
MOTA	528	CB	ARG	Α	125	2.918	29.553	41.593	1.00 26.62
ATOM	529	CG	ARG	Α	125	3.016	30.511	42.783	1.00 30.02
ATOM	530	CD	ARG	Α	125	1.733	31.311	43.002	1.00 32.48
ATOM	531	NE	ARG	Α	125	1.910	32.334	44.034	1.00 36.63
ATOM	532	CZ	ARG	A	125	1.049	33.323	44.282	1.00 38.12
ATOM	533		ARG			-0.070	33.441	43.575	1.00 37.55
ATOM	534		ARG			1.307	34.202	45.240	1.00 38.11
ATOM	535	N	LYS			5189	27.810	39.221	1.00 26.62
ATOM	536	CA	LYS			5.162	26.861	38.079	1.00 26.41
ATOM	537	C	LYS			6.453	26.063	37.986	1.00 24.61
ATOM	538	0	LYS			7.577	26.624	38.141	1.00 22.46
ATOM	539	СВ	LYS			4.971	27.605	36.756	1.00 28.55
ATOM	540		LYS			3.539		36.736	1.00 28.35
		CG					27.804		
ATOM	541	CD	LYS			3.486	28.380	34.917	1.00 36.53
MOTA	542	CE	LYS			2.048	28.607	34.456	1.00 38.52
ATOM	543	NZ	LYS			1.234	27.355	34.550	1.00 40.78
MOTA	544	N	GLY			6.326	24.770	37.731	1.00 23.25
ATOM	545	CA	GLY			7.504	23.941	37.598	1.00 22.82
MOTA	546	С	GLY			7.970	23.995	36.157	1.00 22.77
MOTA	547	0	GLY			7.220	24.487	35.252	1.00 22.00
MOTA	548	N	VAL			9.184	23.521	35.909	1.00 21.58
MOTA	549	CA	VAL			9.731	23.511	34.541	1.00 22.39
MOTA	550	С	VAL			10.736	22.388	34.390	1.00 21.31
MOTA	551	0	VAL			11.547	22.101	35.323	1.00 21.59
MOTA	552	CB	VAL			10.416	24.851	34.180	1.00 21.77
MOTA	553		VAL				25.120	35.122	1.00 22.15
ATOM	554		VAL			10.903	24.809	32.740	1.00 23.66
				••		10.505	24.007	J	23.00

ATOM	555	N	TYR	Α	129	10.700	21.744	33.233	.1.00	21.64
ATOM	556	CA	TYR	Α	129	11.598	20.624	32.933	1.00	21.55
ATOM	557	C	TYR	Α	129	12.298	20.882	31.609	1.00	20.25
MOTA	558	0	TYR	Α	129	11.635	21.188	30.573	1.00	20.01
ATOM	559	CB	TYR	Α	129	10.785	19.333	32.841	1.00	23.37
ATOM	560	CG	TYR	Α	129	11.545	18.164	32.271	1.00	26.64
ATOM	561	CD1				12.628	17.613	32.956	1.00	27.70
ATOM	562	CD2				11.178	17.598	31.048	1.00	27.27
ATOM	563	CE1				13.323	16.529	32.443	1.00	29.33
ATOM	564	CE2	TYR			11.872	16.507	30.524		28.75
ATOM	565	CZ	TYR			12.942	15.980	31.231		28.91
ATOM	566	ОН	TYR			13.634	14.896	30.751		30.21
ATOM	567	N	VAL			13.620	20.782	31.602		19.35
ATOM	568	CA	VAL			14.353	21.003	30.350		17.21
ATOM	569	C	VAL			15.308	19.872	30.022		16.02
	570	0	VAL			16.319	19.628	30.748		16.89
ATOM			VAL			15.136	22.334	30.370		17.86
ATOM	571	CB				15.136	22.485	29.075		15.31
ATOM	572		VAL							15.67
ATOM	573		VAL			14.163	23.505	30.525		
ATOM	574	N	PRO			15.013	19.136	28.945		14.83
ATOM	575	CA	PRO			15.868	18.028	28.529		14.77
ATOM	576	C	PRO			16.743	18.516	27.372		15.00
ATOM	577	0	PRO			16.234	19.154	26.402		15.43
ATOM	578	CB	PRO			14.857	16.971	28.106		13.57
ATOM	579	CG	PRO			13.809	17.806	27.421		13.44
ATOM	580	CD	PRO			13.706	19.078	28.262		13.99
MOTA	581	N	TYR			18.043	18.268	27.465		14.75
MOTA	582	CA	TYR	Α	132	18.989	18.679	26.404		17.37
MOTA	583	С	TYR	A	132	19.438	17.415	25.676	1.00	17.52
MOTA	584	0	TYR			19.100	16.274	26.105		17.41
MOTA	585	СВ	TYR	Α	132	20.211	19.369	27.020	1.00	16.93
ATOM	586	CG	TYR	Α	132	19.909	20.665	27.742	1.00	18.63
MOTA	587	CD1	TYR	Α	132	19.834	21.881	27.051	1.00	17.88
ATOM	588	CD2	TYR	Α	132	19.706	20.681	29.122	1.00	19.01
ATOM	589	CE1	TYR	Α	132	19.564	23.080	27.722	1.00	16.57
ATOM	590	CE2	TYR	Α	132	19.435	21.867	29.799	1.00	17.74
ATOM	591	CZ	TYR	Α	132	19.365	23.062	29.098	1.00	19.02
MOTA	592	OH	TYR	Α	132	19.083	24.229	29.782	1.00	18.23
ATOM	593	N	THR	Α	133	20.188	17.574	24.592	1.00	18.46
MOTA	594	CA	THR	Α	133	20.686	16.403	23.842	1.00	18.54
ATOM	595	С	THR	Α	133	21.525	15.580	24.812	1.00	20.42
ATOM	596	0	THR			21.667	14.325	24.672	1.00	19.49
ATOM	597	СВ	THR	Α	133	21.546	16.846	22.653	1.00	18.40
ATOM	598	OG1	THR	Α	133		17.539	21.708	1.00	20.46
ATOM	599		THR			22.194	15.645	21.976		18.37
ATOM	600	N	GLN			22.064	16.265	25.810		22.23
ATOM	601	CA	GLN			22.890	15.624	26.842		24.27
ATOM	602	C	GLN			22.723	16.406	28.140		23.32
ATOM	603	ō	GLN			23.179	17.580	28.252		21.03
ATOM	604	СВ	GLN			24.352	15.633	26.405		28.22
ATOM	605	CG	GLN			25.140	14.412	26.808		32.76
ATOM	606	CD	GLN			25.020	13.296	25.781		36.63
ATOM	607		GLN			26.052	12.680	25.356		37.34
ATOM	608		GLN			23.791	13.018	25.352		38.92
ATOM	609	NEZ	GLY			22.080	15.789	29.124		23.28
ATOM	610	CA	GLY			21.863	16.460	30.391		21.50
ATOM	611	CA	GLY			20.432	16.946	30.483		22.11
MOTA	612	0	GLY			19.735	17.111	29.435		20.68
ATOM	613	N	LYS			19.733		31.703		22.97
MOTA	614	CA	LYS			18.584	17.190 17.654	31.923		23.80
ATOM	615	CA	LYS			18.429	17.654	33.353		22.33
			LYS					34.269		21.42
MOTA	616	0	пīЭ	A	120	19.196	17.719	34.403	1.00	44.44

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ATOM	617	CB	LYS	A	136		17.606	16.501	31.677	1.00 25.37
ATOM	618	CG	LYS	Α	136		17.823	15.310	32.607	1.00 28.29
ATOM	619	CD	LYS	Α	136		16.804	14.196	32.374	1.00 31.54
ATOM	620	CE			136		16.955	13.570	31.000	1.00 34.21
ATOM	621	NZ			136		15.996	12.444	30.789	1.00 37.76
MOTA	622	N			137		17.470	19.040	33.573	1.00 21.02
MOTA	623	ÇA	TRP	Α	137		17.214	19.562	34.928	1.00 20.75
ATOM	624	С	TRP	Α	137		15.750	19.907	35.133	1.00 20.62
ATOM	625	ō			137		14.951	19.978	34.153	1.00 20.05
ATOM	626	CB			137		18.077	20.800	35.231	1.00 18.46
MOTA	627	CG			137		17.960	21.937	34.248	1.00 18.02
ATOM	628	CD1	TRP	Α	137		18.865	22.276	33.281	1.00 18.12
MOTA	629	CD2	TRP	Α	137		16.881	22.879	34.134	1.00 17.27
MOTA	630		TRP				18.419	23.369	32.574	1.00 17.78
		CE2	TRP							
MOTA	631						17.204	23.758	33.074	1.00 17.40
MOTA	632	CE3			137		15.675	23.067	34.823	1.00 17.08
MOTA	633	CZ2	TRP	Α	137		16.363	24.807	32.684	1.00 15.50
ATOM	634	CZ3	TRP	Α	137		14.836	24.113	34.434	1.00 17.23
ATOM	635	CH2	TRP	А	137	•	15.188	24.968	33.373	1.00 17.46
ATOM	636	N			138		15.385	20.098	36.395	1.00 21.53
MOTA	637	CA			138		14.014	20.472	36.789	1.00 24.94
ATOM	638	С	GLU	Α	138		14.166	21.642	37.745	1.00 23.18
ATOM	639	0	GLU	Α	138		15.168	21.719	38.526	1.00 21.21
ATOM	640	СВ	GLU	А	138		13.320	19.320	37.515	1.00 28.46
ATOM	641	CG			138		13.053	18.101	36.656	1.00 34.91
ATOM	642	CD	GLU				12.562	16.919	37.472	1.00 37.93
ATOM	643		GLU				12.175	15.897	36.864	1.00 40.28
ATOM	644	OE2	GLU	Α	138		12.570	17.009	38.722	1.00 40.20
ATOM	645	N	GLY	Α	139		13.214	22.559	37.711	1.00 22.13
MOTA	646	CA	GLY	А	139		13.298	23.693	38.604	1.00 22.60
ATOM	647	C	GLY				11.975	24.402	38.713	1.00 21.54
MOTA	648	0	GLY				10.949	23.953	38.116	1.00 23.29
ATOM	649	N	GĽŰ	Α	140		11.962	25.494	39.465	1.00 21.74
MOTA	650	CA	GLU	Α	140		10.733	26.284	39.648	1.00 21.81
ATOM	651	С	GLU	Α	140		10.900	27.646	38.998	1.00 19.04
ATOM	652	Ö			140		11.975	28.304	39.125	1.00 18.42
	653					•				
MOTA		CB	GLU				10.404	26.425	41.139	1.00 24.39
ATOM	654	CG	GLU				11.479	25.887	42.065	1.00 28.61
MOTA	655	CD	GLU	Α	140		10.922	25.385	43.383	1.00 29.72
ATOM	656	OE1	GLU	A	140		10.311	24.297	43.389	1.00 31.43
ATOM	657	OE2	GLU	Α	140		11.091	26.077	44.410	1.00 30.48
ATOM	658	N	LEU				9.870	28.071	38.278	1.00 16.35
	659	CA								
MOTA			LEU				9.901	29.360	37.585	1.00 15.48
MOTA	660	С	LEU				9.674	30.546	38.511	1.00 15.68
MOTA	661	0	LEU	Α	141		8.832	30.499	39.466	1.00 13.45
MOTA	662	CB ·	LEU	A	141		8.864	29.376	36.460	1.00 15.23
MOTA	663	CG	LEU				9.145	28.412	35.300	1.00 16.27
MOTA	664		LEU				8.008	28.461	34.300	1.00 15.60
MOTA	665		LEU				10.458	28.785	34.627	1.00 16.48
MOTA	666	N	GLY				10.424	31.608	38.241	1.00 15.15
MOTA	667	CA	GLY	Α	142		10.323	32.819	39.015	1.00 12.33
MOTA	668	С	GLY	Α	142		10.845	33.953	38.167	1.00 14.67
ATOM	669	0	GLY				11.242	33.758	36.971	1.00 13.75
ATOM	670	N	THR				10.877		38.754	
								35.137		1.00 14.88
ATOM	671	CA	THR				11.354	36.324	38.050	1.00 15.26
MOTA	672	С	THR				12.262	37.103	39.008	1.00 14.53
ATOM	673	0	THR	Α	143		12.119	36.991	40.269	1.00 13.46
ATOM	674	CB	THR				10.131	37.154	37.600	1.00 16.18
ATOM	675		THR				10.192	37.362	36.187	1.00 20.69
ATOM	676		THR							
							10.058	38.465	38.325	1.00 12.43
MOTA	677	N	ASP				13.202	37.866	38.466	1.00 14.22
ATOM	678	CA	ASP	A	144		14.117	38.652	39.321	1.00 15.38

ATOM	679	С	ASP A	144	14.942	39.609	38.479	1.00 15.67
ATOM	680	0	ASP A		14.984	39.496	37.208	1.00 16.83
ATOM	681	СВ	ASP A	144	15.063	37.721	40.086	1.00 15.20
ATOM	682	CG	ASP A	144	15.367	38.218	41.496	1.00 17.84
ATOM	683	OD1	ASP A		15.359	39.447	41.724	1.00 16.62
ATOM	684		ASP A		15.630	37.373	42.379	1.00 16.33
ATOM	685	N	LEU A		15.596	40.551	39.147	1.00 16.74
ATOM	686	CA	LEU A		16.442	41.537	38.454	1.00 18.66
ATOM	687	C	LEU A		17.757	40.854	38.101	1.00 20.21
ATOM	688	ō	LEU A		18.381	40.147	38.961	1.00 21.75
ATOM	689	CB	LEU A		16.697	42.746	39.351	1.00 18.43
ATOM	690	CG	LEU A		15.452	43.522	39.786	1.00 19.69
ATOM	691		LEU A		15.878	44.720	40.628	1.00 19.11
ATOM	692	_	LEU A		14.660	43.971	38.557	1.00 18.50
ATOM	693	N	VAL A		18.186	41.030	36.858	1.00 20.48
ATOM	694	CA	VAL A		19.426	40.402	36.387	1.00 21.21
ATOM	695	C	VAL A		20.331	41.426	35.725	1.00 22.80
ATOM	696	0	VAL A		19.849	42.386	35.045	1.00 22.16
MOTA	697	CB	VAL A		19.118	39.265	35.373	1.00 20.39
MOTA	698	CG1			20.405	38.575	34.941	1.00 20.39
ATOM	699	CG2	VAL A		18.163	38.261	35.998	1.00 17.90
ATOM	700	N	SER A		21.633	41.251	35.913	1.00 22.35
ATOM	701	CA	SER A		22.615	42.158	35.309	1.00 23.39
ATOM	702	C	SER A		23.829	41.383	34.833	1.00 21.77
MOTA	702	0	SER A		24.119	40.242	35.321	1.00 20.08
ATOM	704	СВ	SER A		23.059	43.225	36.316	1.00 25.41
MOTA	705	OG	SER A		21.993	44.107	36.627	1.00 31.97
MOTA	706	И	ILE A		24.534	41.972	33.878	1.00 19.69
ATOM	707	CA	ILE A		25.757	41.377	33.329	1.00 19.14
ATOM	708	C	ILE A		26.853	42.405	33.614	1.00 18.85
ATOM	709	Ö	ILE A		27.021	43.408	32.853	1.00 17.87
MOTA	710	СВ	ILE F		25.618	41.137	31.817	1.00 18.61
MOTA	711	CG1	ILE A		24.449	40.181	31.559	1.00 19.01
MOTA	712	CG2	ILE A		26.909	40.564	31.255	1.00 17.68
MOTA	713	CD1			24.221	39.864	30.097	1.00 19.61
MOTA	714	N	PRO F		27.601	42.214	34.711	1.00 17.99
ATOM	715	CA	PRO F		28.679	43.134	35.095	1.00 21.17
MOTA	716	C	PRO Z		29.523	43.638	33.926	1.00 22.18
ATOM	717	Ö	PRO F		29.800	44.869	33.823	1.00 24.08
ATOM	718	СВ	PRO I		29.485	42.317	36.103	1.00 19.87
MOTA	719	CG	PRO I		28.404	41.529	36.797	1.00 19.57
ATOM	720	CD		149	27.542	41.061	35.628	1.00 17.55
ATOM	721	N	HIS A		29.930	42.733	33.041	1.00 23.43
ATOM	722	CA	HIS A		30.748	43.119	31.869	1.00 23.84
ATOM	723	C	HIS A		29.933	43.067	30.588	1.00 24.47
ATOM	724	0	HIS A		30.334	42.431	29.566	1.00 25.89
ATOM	725	СВ	HIS A		31.968	42.211	31.765	1.00 23.54
ATOM	726	CG	HIS A		32.880	42.313	32.945	1.00 26.15
ATOM	727		HIS A		33.619	43.446	33.216	1.00 27.28
ATOM	728		HIS A		33.149	41.439	33.943	1.00 26.32
ATOM	729		HIS A		34.305	43.264	34.330	1.00 27.48
ATOM	730		HIS A		34.038	42.055	34.791	1.00 28.01
	731	NEZ	GLY 2		28.785	43.727	30.630	1.00 25.49
ATOM ATOM	732	CA	GLY 2		27.906	43.784	29.485	1.00 26.41
ATOM	732	C	GLY A		27.325	45.179	29.468	1.00 27.16
	734	0	GLY A		27.323	46.136	29.983	1.00 26.97
ATOM	735	N	PRO 2		26.125	45.370	28.903	1.00 28.12
ATOM ATOM	736	CA	PRO Z		25.540	46.712	28.880	1.00 28.75
	737	C	PRO A		25.219	47.165	30.304	1.00 30.53
MOTA	73 <i>7</i> 738	0	PRO A		24.844	46.331	31.182	1.00 28.62
ATOM ATOM	739	СВ	PRO A		24.294	46.528	28.017	1.00 29.49
ATOM	740	CG	PRO Z		23.897	45.105	28.303	1.00 29.85
AION	,40	CG	110 /	. 132	23.031	-J. LVJ	20.505	

MOTA	741	CD	PRO	Α	152		25.227	44.385	28.277	1.00 28.	15
ATOM	742	N	ASN	Α	153		25.375	48.457	30.560	1.00 33.	በ፯
ATOM	743	CA			153						
							25.111	49.016	31.902	1.00 34.	
MOTA	744	С	ASN	Α	153		23.604	49.096	32.144	1.00 33.	81
ATOM	745	0	ASN	Α	153		23.009	50.218	32.222	1.00 33.	63
ATOM	746	СВ			153		25.755	50.401	32.009	1.00 37.	
MOTA	747	CG	ASN	Α	153		25.680	50.978	33.406	1.00 38.	88
MOTA	748	OD1	ASN	Α	153		25:974	50.272	34.416	1.00 40.	17
ATOM	749	ND2					25.309	52.251	33.504	1.00 39.	
MOTA	750	И			154		22.971	47.934	32.265	1.00 31.	
MOTA	751	CA	VAL	Α	154		21.514	47.872	32.486	1.00 29.	59
ATOM	752	С	VAT.	Δ	154		21.113	46.739	33.418	1.00 29.	
ATOM	753	0			154		21.924	45.809	33.718	1.00 30.	
ATOM	754	CB	VAL	Α	154		20.755	47.681	31.154	1.00 29.	95
ATOM	755	CG1	VAL	Α	154		20.990	48.875	30.242	1.00 29.	70
ATOM	756	CG2	VAL				21.216	46.397	30.474	1.00 28.	
MOTA	757	N	THR				19.874	46.799	33.882	1.00 27.	83
MOTA	758	CA	THR	Α	155		19.323	45.773	34.779	1.00 27.	61
ATOM	759	С	THR	A	155		17.918	45.472	34.296	1.00 26.	Ω 1
ATOM	760	ō	THR				17.114	46.413	34.041	1.00 27.	
ATOM	761	CB	THR	A	155		19.268	46.280	36.229	1.00 27.	24
ATOM	762	OG1	THR	Α	155		20.603	46.486	36.703	1.00 29.	54
ATOM	763	CG2	THR				18.573	45.270	37.129	1.00 27.	
MOTA	764	N	VAL				17.592	44.197	34.143	1.00 24.	
ATOM	765	CA	VAL	A	156		16.241	43.847	33.672	1.00 24.	32
MOTA	766	С	VAL	Α	156		15.631	42.736	34.504	1.00 23.	23
ATOM	767	Ō	VAL				16.364	41.920	35.154	1.00 23.	
· MOTA	768	СВ	VAL	Α	156		16.253	43.402	32.184	1.00 25.	34
MOTA	769	CG1	VAL	Α	156		17.178	44.302	31,379	1.00 26.	63
ATOM	770	CG2	VAL	Δ	156		16.684	41.960	32.063	1.00 24.	
MOTA	771	Ν.			157	•	14.306	42.687	34.521	1.00 21.	
ATOM	772	CA	ARG	Α	157		13.613	41.626	35.262	1.00 20.	90
ATOM	773	C	ARG	А	157		13.374	40.560	34.215	1.00 20.	13
ATOM	774	ō	ARG				12.746	40.836	33.152		
										1.00 19.	
ATOM	775	CB	ARG	Α	157		12.280	42.121	35.830	1.00 20.	03
ATOM	776	CG	ARG	Α	157		11.528	41.053	36.621	1.00 18.	95
ATOM	777	CD	ARG			•	10.271	41.616	37.260	1.00 18.	
	778										
ATOM		NE	ARG				10.554	42.408	38.456	1.00 18.	
ATOM	779	CZ	ARG	Α	157		10.973	41.902	39.613	1.00 19.	19
ATOM	780	NH1	ARG	A	157		11.167	40.596	39.747	1.00 18.	30
ATOM	781	NH2					11.178	42.703	40.650	1.00 15.	
MOTA	782	N	ALA				13.878	39.359	34.463	1.00 20.	
ATOM	783	CA	ALA	Α	158		13.713	38.266	33.496	1.00 19.	80
ATOM	784	С	ALA	Α	158		13.279	36.986	34.175	1.00 19.	45
ATOM	785	0	ALA				13.379	36.845	35.432	1.00 19.	
MOTA	786	СВ	ALA				15.017	38.031	32.756	1.00 18.	
ATOM	787	N	ASN	Α	159		12.792	36.053	33.370	1.00 18.	80
ATOM	788	CA	ASN	Α	159		12.363	34.756	33.876	1.00 18.	21
ATOM	789	C	ASN				13.607	33.992	34.282	1.00 18.	
ATOM	790	0	ASN				14.666	34.033	33 . 577	1.00 19.	42
ATOM	791	CB	ASN	Α	159		11.601	33.992	32.797	1.00 16.	91
ATOM	792	CG	ASN	Α	159		10.282	34.647	32.459	1.00 18.	46
MOTA	793		ASN				9.479	34.978	33.381	1.00 19.	
MOTA	794	ND2	ASN	Α	159		10.020	34.848	31.174	1.00 16.	51
MOTA	795	N	ILE	A	160		13.518	33.311	35.412	1.00 18.	73
ATOM	796	CA	ILE				14.643	32.529	35.916	1.00 17.	
MOTA	797	С	ILE				14.112	31.191	36.373	1.00 19.	
MOTA	798	0	ILE	Α	160		13.122	31.125	37.176	1.00 18.	38
ATOM	799	CB	ILE				15.319	33.212	37.128	1.00 18.	36
ATOM	800	CG1	ILE				15.764	34.629	36.758	1.00 17.	
MOTA	801	CG2	ILE				16.521	32.394	37.585	1.00 17.	
MOTA	802	CD1	ILE	Α	160		16.521	35.336	37.875	1.00 18.	56

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MOTA	803	N			161	14.717	30.123	35.871	1.00 17.55
MOTA	804	CA	ALA	Α	161	14.314	28.778	36.275	1.00 18.11
ATOM	805	С	ALA	Α	161	15.267	28.394	37.399	1.00 18.26
ATOM	806	Ō			161	16.507	28.223	37.166	1.00 17.61
ATOM	807	CB			161	14.447	27.805	35.105	1.00 17.28
ATOM	808	N	ALA	Α	162	14.737	28.283	38.614	1.00 17.99
MOTA	809	CA	ALA	Α	162	15.567	27.901	39.775	1.00 18.02
ATOM	810	C	ΔΤ.Δ	Δ	162	15.746	26.382	39.774	1.00 18.52
ATOM	811	0			162	14.835	25.619	40.207	1.00 18.43
MOTA	812	CB			162	14.897	28.359	41.067	1.00 17.36
ATOM	813	И	ILE	Α	163	16.900	25.928	39.300	1.00 19.89
ATOM	814	CA	ILE	Α	163	17.204	24.480	39.215	1.00 18.56
ATOM	815	C			163	17.314	23.802	40.577	1.00 20.34
MOTA	816	0			163	18.238	24.122	41.402	1.00 19.83
MOTA	817	CB	ILE	Α	163	18.512	24.245	38.430	1.00 17.19
MOTA	818	CG1	ILE	Α	163	18.347	24.753	36.994	1.00 16.02
ATOM	819	CG2			163	18.874	22.761	38.445	1.00 14.93
ATOM	820	CD1			163	19.628	24.735	36.174	1.00 16.24
MOTA	821	N			164	16.409	22.860	40.826	1.00 20.42
ATOM	822	CA	THR	Α	164	16.379	22.122	42.112	1.00 23.01
ATOM	823	С	THR	Α	164	16.817	20.665	41.958	1.00 24.30
MOTA	824	0	THR	Δ	164	17.119	19.966	42.973	1.00 26.25
ATOM	825				164	14.966	22.173	42.735	1.00 22.01
		CB							
ATOM	826	OG1	THR	A	164	13.990	21.799	41.754	1.00 22.15
MOTA	827	CG2	THR	Α	164	14.656	23.584	43.214	1.00 22.73
ATOM	828	N	GLU	Α	165	16.858	20.187	40.721	1.00 25.84
ATOM	829	CA			165	17.281	18.804	40.444	1.00 27.82
ATOM	830	C			165	17.800	18.693	39.024	1.00 26.80
MOTA	831	0	GLU			17.246	19.323	38.072	1.00 26.59
ATOM	832	CB	GLU	Α	165	16.121	17.834	40.678	1.00 31.67
ATOM	833	CG	GLU	Α	165	16.233	17.118	42.020	1.00 38.94
MOTA	834	CD	GLU			14.913	16.568	42.519	1.00 41.54
MOTA	835		GLU			14.282	15.765	41.796	1.00 44.35
MOTA	836	OE2	GLU			14.510	16.940	43.644	1.00 43.84
ATOM	837	N	SER	Α	166	18.861	17.919	38.852	1.00 24.81
ATOM	838	CA	SER	Α	166	19.455	17.765	37.525	1.00 25.32
ATOM	839	C	SER			20.213	16.459	37.397	1.00 25.44
MOTA	840	0	SER			20.551	15.795	38.427	1.00 24.00
ATOM	841	CB	SER	Α	166	20.405	18.928	37.255	1.00 23.13
ATOM	842	OG	SER	Α	166	21.444	18.939	38.217	1.00 21.22
ATOM	843	N	ASP	А	167	20.490	16.079	36.155	1.00 26.01
MOTA	844	CA	ASP			21.227	14.842	35.871	1.00 26.62
ATOM	845	C	ASP			22.138	15.038	34.671	1.00 25.62
MOTA	846	0	ASP			21.656	15.300	33.528	1.00 24.35
ATOM	847	CB	ASP	Α	167	20.253	13.691	35.601	1.00 30,53
ATOM	848	CG	ASP	Α	167	20.966	12.370	35.387	1.00 32.67
ATOM	849		ASP			21.912	12.083	36.152	1.00 36.14
	850		ASP						
MOTA						20.586	11.615	34.469	1.00 34.63
ATOM	851	N	LYS	Α	168	23.440	14.930	34.910	1.00 25.32
ATOM	852	CA	LYS	Α	168	24.461	15.078	33.847	1.00 25.94
MOTA	853	С	LYS	Α	168	24.416	16.445	33.175	1.00 25.49
MOTA	854	0	LYS			24.742	16.580	31.955	1.00 25.50
MOTA	855	CB	LYS			24.282	13.979	32.800	1.00 27.68
MOTA	856	CG	LYS			24.408	12.570	33.362	1.00 30.33
MOTA	857	CD	LYS	Α	168	24.117	11.532	32.292	1.00 32.36
MOTA	858	CE	LYS			24.205	10.126	32.855	1.00 34.37
ATOM	859	NZ	LYS			23.889	9.101	31.821	1.00 36.50
	860	N							
MOTA			PHE			24.024	17.460	33.937	1.00 22.87
MOTA	861	CA	PHE			23.942	18.835	33.418	1.00 20.96
MOTA	862	C	PHE	Α	169	25.158	19.616	33.897	1.00 22.06
MOTA	863	0	PHE	Α	169	25.983	20.119	33.069	1.00 20.71
MOTA	864	СВ	PHE			22.668	19.506	33.919	1.00 19.76
				.,	_05	22.000	19.000	JJ.JLJ	2.00 25.70

MOTA	865	CG	PHE A	169	22.526	20.931	33.479	1.00 18.95
ATOM	866	CD1	PHE A	169	22.400	21.248	32.130	1.00 18.27
ATOM	867	CD2	PHE A	169	22.525	21.963	34.416	1.00 18.36
ATOM	868	CE1			22.275	22.571		
							31.720	1.00 16.94
ATOM	869	CE2			22.401	23.287	34.013	1.00 17.25
ATOM	870	\mathbf{cz}	PHE A		22.275	23.590	32.661	1.00 16.89
ATOM	871	N	PHE A	170	25.292	19.738	35.212	1.00 20.46
ATOM	872	CA	PHE A	170	26.438	20.452	35.788	1.00 21.45
ATOM	873	С	PHE A		27.702	19.620	35.574	1.00 22.40
ATOM	874	ŏ	PHE A		27.675	18.355	35.665	1.00 22.55
ATOM	875	СВ	PHE A					
					26.205	20.705	37.281	1.00 19.44
ATOM.	876	CG	PHE A		25.079	21.663	37.559	1.00 18.44
ATOM	877	CD1	PHE A		23.988	21.276	38.330	1.00 18.45
ATOM	878	CD2	PHE A	170	25.098	22.948	37.025	1.00 16.73
ATOM	879	CE1	PHE A	170	22.932	22.154	38.563	1.00 17.50
ATOM	880	CE2	PHE A	170	24.046	23.832	37.253	1.00 17.78
ATOM	881	CZ	PHE A		22.963	23.432	38.023	1.00 16.39
ATOM	882	N	ILE A		28.805	20.297	35.272	
								1.00 23.10
ATOM	883	CA	ILE A		30.095	19.615	35.043	1.00 22.87
MOTA	884	С	ILE A		31.057	19.962	36.163	1.00 24.02
ATOM	885	0	ILE A	171	31.222	21.162	36.537	1.00 22.48
MOTA	886	CB	ILE A	171	30.729	20.048	33.704	1.00 24.70
MOTA	887	CG1	ILE A	171	29.823	19.632	32.544	1.00 22.57
ATOM	888	CG2	ILE A		32.123	19.434	33.558	1.00 22.35
ATOM	889	CD1			30.319	20.100	31.192	1.00 23.46
MOTA	890	N	ASN A		31.702			
ATOM						18.942	36.709	1.00 27.12
	891	CA	ASN A		32.657	19.143	37.809	1.00 30.01
ATOM	892	С	ASN A		33.864	19.975	37.359	1.00 29.57
MOTA	893	0	ASN A	172	34.616	19.574	36.418	1.00 29.20
MOTA	894	CB	ASN A	172	33.105	17.779	38.337	1.00 31.92
ATOM	895	CG	ASN A	1.72	33.913	17.885	39.608	1.00 34.74
ATOM	896	OD1			33.615	18.737	40.504	1.00 36.04
ATOM	897	ND2	ASN A		34.927	17.034	39.734	1.00 36.14
ATOM	898	N	GLY A					
					34.049	21.132	37.991	1.00 28.24
ATOM	899	CA	GLY A		35.166	22.001	37.659	1.00 27.99
ATOM	900	C	GLY A		34.973	22.938	36.476	1.00 28.87
ATOM	901	0	GLY A	173	35.944	23.644	36.063	1.00 29.20
ATOM	902	N	SER A	174	33.769	22.988	35.914	1.00 28.95
ATOM	903	CA	SER A	174	33.498	23.880	34.748	1.00 29.13
ATOM	904	С	SER A	174	33.524	25.348	35.168	1.00 27.92
ATOM	905	0	SER A		33.878	26.255	34.354	1.00 29.51
ATOM	906	СВ	SER A		32.130	23.562		
ATOM	907	OG	SER A				34.148	1.00 28.90
					31.102	23.922	35.054	1.00 30.49
MOTA	908	N	ASN A		33.140	25.593	36.416	1.00 25.45
ATOM	909	CA	ASN A		33.095	26.951	37.011	1.00 23.59
ATOM	910	C	ASN A	175	31.855	27.767	36.647	1.00 21.71
ATOM	911	0	ASN A	175	31.828	29.019	36.853	1.00 20.11
MOTA	912	СВ	ASN A	175	34.354	27.754	36.662	1.00 27.01
ATOM	913	CG	ASN A		34.548	28.950	37.582	1.00 29.09
ATOM	914		ASN A		34.648			
ATOM	915					28.794	38.840	1.00 30.19
			ASN A		34.600	30.144	37.004	1.00 30.01
ATOM	916	N	TRP A		30.841	27.121	36.078	1.00 16.70
ATOM	917	CA	TRP A		29.590	27.847	35.790	1.00 18.41
MOTA	918	С	TRP A		28.482	27.170	36.580	1.00 17.87
MOTA	919	0	TRP A	176	28.534	25.927	36.838	1.00 15.45
MOTA	920	СВ	TRP A		29.248	27.888	34.292	1.00 16.48
ATOM	921	CG	TRP A		29.257	26.588	33.563	1.00 17.63
ATOM	922		TRP A		30.291	26.063	32.842	1.00 17.03
ATOM	923		TRP A		28.165			
						25.668	33.425	1.00 17.78
ATOM	924		TRP A		29.911	24.881	32.258	1.00 16.01
ATOM	925		TRP A		28.612	24.613	32.599	1.00 16.95
ATOM	926	CE3	TRP A	176	26.852	25.635	33.918	1.00 18.29

MOTA	927	CZ2	TRP A	176	27.794	23.532	32.252	1.00 17.40
ATOM	928	CZ3	TRP A	176	26.034	24.557	33.573	1.00 19.02
ATOM	929	CH2	TRP A	176	26.512	23.521	32.747	1.00 19.06
ATOM	930		GLU A		27.496	27.950	37.005	1.00 18.68
							37.797	
ATOM	931	CA	GLU A		26.387	27.385		1.00 21.01
ATOM	932	С	GLU A		25.024	27.700	37.224	1.00 20.81
MOTA	933	0	GLU A	177	23.977	27.582	37.938	1.00 21.08
ATOM	934	СВ	GLU A	177	26.461	27.869	39.250	1.00 22.84
ATOM	935	CG	GLU A		26.865	29.322	39.443	1.00 26.63
					28.377		39.446	1.00 27.90
MOTA	936	CD	GLU A			29.531		
MOTA	937	OE1			29.121	28.568	39.726	1.00 28.44
MOTA	938	OE2	GLU A	177	28.818	30.670	39.186	1.00 28.24
ATOM	939	N	GLY A	178	25.007	28.088	35.953	1.00 18.48
ATOM	940	CA	GLY A	178	23.759	28.411	35.295	1.00 16.82
ATOM	941	C	GLY A		23.929	28.406	33.791	1.00 15.90
							33.264	
MOTA	942	0	GLY A		25.070	28.248		1.00 15.75
MOTA	943	N	ILE A	179	22.831	28.589	33.076	1.00 14.53
MOTA	944	CA	ILE A	179	22.882	28.588	31.610	1.00 14.26
ATOM	945	С	ILE A	179	22.007	29.701	31.057	1.00 14.53
MOTA	946	Ō	ILE A		20.896	29.980	31.603	1.00 15.23
	947	СВ	ILE A		22.428	27.217	31.069	1.00 14.45
ATOM								
ATOM	948	CG1			22.535	27.183	29.548	1.00 14.28
ATOM	949	CG2	ILE A	179	21.002	26.921	31.525	1.00 13.41
MOTA	950	CD1	ILE A	179	22.359	25.788	28.974	1.00 13.85
ATOM	951	N	LEU A	180	22.489	30.350	29.998	1.00 14.91
ATOM	952	CA	LEU A		21.763	31.464	29.353	1.00 14.24
					21.311	31.050	27.961	1.00 15.19
MOTA	953	C	LEU A					
MOTA	954	Ο.	LEU A		22.117	31.115	26.973	1.00 15.79
ATOM	955	CB	LEU A	180	22.675	32.690	29.223	1.00 14.83
ATOM	956	CG	LEU A	180	22.078	34.107	29.257	1.00 16.59
MOTA	957		LEU A		22.902	34.996	28.351	1.00 15.04
ATOM	958		LEU A		20.622	34.120	28.818	1.00 17.08
MOTA	959	N	GLY A		20.057	30.621	27.851	1.00 15.40
MOTA	960	CA	GLY A	. 181	19.525	30.227	26.561	1.00 13.68
ATOM	961	C	GLY A	181	19.276	31.481	25.741	1.00 15.03
ATOM	962	0	GLY A	181	18.402	32.330	26.107	1.00 14.58
ATOM	963	N			20.002	31.629	24.638	1.00 12.84
ATOM	964	CA	LEU A		19.859	32.831	23.787	1.00 13.53
					19.029			1.00 14.25
MOTA	965	C	LEU A			32.646	22.521	
MOTA	966	0	LEU A		18.883	33.607	21.701	1.00 13.52
MOTA	967	CB	LEU A	182	21.250	33.352	23.418	1.00 13.44
MOTA	968	CG	LEU A	182	22.036	33.949	24.583	1.00 11.84
ATOM	969	CD1	LEU A	182	23.506	34.067	24.211	1.00 11.17
ATOM	970		LEU A			35.311	24.936	1.00 12.14
	971	-			18.491	31.449	22.322	1.00 15.12
MOTA		N	ALA A					
MOTA	972	CA	ALA A		17.660	31.183	21.131	1.00 15.16
MOTA	973	С	ALA A		16.276	31.788	21.361	1.00 17.66
MOTA	974	0	ALA A	183	16.053	32.526	22.377	1.00 16.26
MOTA	975	СВ	ALA A	183	17.557	29.684	20.875	1.00 14.23
ATOM	976	N	TYR A		15.338	31.487	20.466	1.00 18.41
MOTA	977	CA	TYR A		13.976	32.060	20.550	1.00 17.40
								1.00 17.40
MOTA	978	C	TYR A		12.953	31.334	21.424	
ATOM	979	0	TYR A		13.131	30.135	21.807	1.00 14.95
MOTA	980	CB	TYR A	184	13.411	32.237	19.138	1.00 18.07
MOTA	981	CG	TYR A	184	14.327	33.017	18.216	1.00 19.50
ATOM	982	CD1			15.295	32.367	17.446	1.00 19.23
ATOM	983	CD2			14.233	34.408	18.119	1.00 19.65
								1.00 19.22
MOTA	984		TYR A		16.144	33.083	16.599	
MOTA	985	CE2	TYR A		15.079	35.134	17.279	1.00 19.50
MOTA	986	CZ	TYR A	. 184	16.027	34.466	16.521	1.00 19.86
MOTA	987	OH	TYR A	184	16.842	35.185	15.670	1.00 20.69
ATOM	988	N	ALA A	. 185	11.873	32.046	21.734	1.00 16.29

MOTA	989	CA	ALA A	185	10.784	31.519	22.592	1.00 17.90
MOTA	990	С	ALA A	185	10.185	30.221	22.068	1.00 17.38
	991	ō	ALA A		9.682	29.372	22.869	1.00 15.41
MOTA								
MOTA	992	CB	ALA A		9.690	32.579	22.742	1.00 15.99
MOTA	993	N	GLU A	186	10.232	30.046	20.751	1.00 20.56
MOTA	994	CA	GLU A	186	9.679	28.846	20.086	1.00 23.43
ATOM	995	С	GLU A		10.169	27.533	20.690	1.00 23.87
					**		20.619	1.00 24.67
ATOM	996	0	GLU A		9.448	26.486		
MOTA	997	CB	GLU A	186	10.009	28.887	18.591	1.00 27.60
MOTA	998	CG	GLU A	186	9.447	27.729	17.786	1.00 32.42
ATOM	999	CD	GLU A	186	7.941	27.593	17.923	1.00 36.08
ATOM	1000	OE1			7.255	28.633	18.041	1.00 39.03
							17.900	
MOTA	1001	OE2			7.439	26.448		1.00 37.05
MOTA	1002	N	ILE A	187	11.363	27.540	21.283	1.00 22.31
ATOM	1003	CA	ILE A	187	11.904	26.302	21.900	1.00 19.35
MOTA	1004	С	ILE A	187	12.113	26.441	23.403	1.00 20.13
ATOM	1005	Ō	ILE A		12.887	25.654	24.034	1.00 19.35
	1006	СВ	ILE A		13.241	25.872	21.248	1.00 19.03
MOTA								
ATOM	1007	CG1			14.270	26.998	21.355	1.00 18.36
ATOM	1008	CG2	ILE A	187	13.008	25.488	19.795	1.00 19.03
ATOM	1009	CD1	ILE A	187	15.627	26.635	20.780	1.00 17.45
MOTA	1010	N	ALA A	188	11.441	27.416	23.999	1.00 19.82
ATOM	1011	CA	ALA A		11.551	27.636	25.454	1.00 20.35
MOTA	1012	С	ALA A		10.622	26.661	26.171	1.00 19.60
MOTA	1013	0	ALA A	188	9.554	26.277	25.618	1.00 19.52
ATOM	1014	CB	ALA A	188	11.160	29.083	25.793	1.00 17.16
MOTA	1015	N	ARG A	189	11.004	26.231	27.372	1.00 20.77
ATOM	1016	CA	ARG A	189	10.142	25.324	28.164	1.00 21.43
	1017	C	ARG A		9.577	26.162	29.303	1.00 22.80
MOTA								
MOTA	1018	0	ARG A		10.274	27.099	29.817	1.00 23.68
ATOM	1019	CB	ARG A	189	10.949	24.151	28.753	1.00 22.36
ATOM	1020	CG	ARG A	189	11.689	23.285	27.729	1.00 23.90
MOTA	1021	CD	ARG A	189	10.765	22.818	26.624	1.00 24.33
ATOM	1022	NE	ARG A		11.419	21.914	25.681	1.00 25.35
MOTA	1023	CZ	ARG A		11.336	20.586	25.724	1.00 27.35
MOTA	1024	NH1	ARG A		10.620	19.991	26.673	1.00 24.73
ATOM	1025	NH2	ARG A	189	11.959	19.849	24.807	1.00 25.42
MOTA	1026	N	PRO A	190	8.325	25.890	29.725	1.00 23.27
ATOM	1027	CA	PRO A	190	7.442	24.830	29.216	1.00 23.21
MOTA	1028	C	PRO A		6.826	25.110	27.849	1.00 23.72
	1029						27.101	1.00 23.72
MOTA		0	PRO A		6.458	24.157		
MOTA	1030	CB	PRO A		6.377	24.713	30.305	1.00 22.63
MOTA	1031	CG	PRO A	190	6.285	26.115	30.830	1.00 24.33
MOTA	1032	CD	PRO A	190	7.745	26.527	30.921	1.00 22.73
ATOM	1033	N	ASP A		6.681	26.383	27.508	1.00 25.20
MOTA	1034	CA	ASP A		6.107	26.754	26.202	1.00 25.89
ATOM	1035	C	ASP A		6.653	28.106	25.770	1.00 25.76
MOTA	1036	0	ASP A		7.488	28.716	26.498	1.00 24.40
MOTA	1037	CB	ASP A	191	4.569	26.757	26.269	1.00 28.36
ATOM	1038	CG	ASP A	191	4.024	27.697	27.323	1.00 30.16
MOTA	1039	OD1	ASP A		2.887	27.468	27.783	1.00 33.88
MOTA	1040		ASP A		4.714	28.669	27.686	1.00 30.53
								1.00 26.01
MOTA	1041	N	ASP A		6.214	28.596	24.617	
MOTA	1042	CA	ASP A		6.724	29.877	24.088	1.00 26.22
MOTA	1043	С	ASP A	192	6.236	31.123	24.813	1.00 26.52
MOTA	1044	0	ASP A	192	6.567	32.275	24.395	1.00 26.27
ATOM	1045	СВ	ASP A		6.419	29.985	22.589	1.00 27.69
ATOM	1045	CG	ASP A			30.161	22.296	1.00 29.61
					4.940			
ATOM	1047		ASP A		4.102	29.647	23.066	1.00 31.87
MOTA	1048	OD2			4.618	30.805	21.279	1.00 30.31
MOTA	1049	N	SER A	193	5.470	30.947	25.885	1.00 24.46
ATOM	1050	CA	SER A	193	4.988	32.117	26.645	1.00 24.21

MOTA	1051	С	SER A	193	6.078	32.565	27.614	1.00 22.68
MOTA	1052	0	SER A		6.082	33.740	28.082	1.00 22.41
ATOM	1053	CB	SER A	193	3.701	31.787	27.415	1.00 25.67
MOTA	1054	OG	SER A	193	3.910	30.774	28.386	1.00 27.13
	1055		LEU A		7.009	31.670	27.932	1.00 20.84
MOTA		N						
ATOM	1056	CA	LEU A	194	8.107	32.044	28.852	1.00 18.87
ATOM	1057	С	LEU A	194	9.149	32.830	28.065	1.00 18.82
		ō	LEU A		10.066	32.240	27.419	1.00 19.19
ATOM	1058							
ATOM	1059	СВ	LEU A	194	8.758	30.809	29.469	1.00 17.48
ATOM	1060	CG	LEU A	194	9.680	31.201	30.631	1.00 19.18
ATOM	1061	CD1	LEU A	194	8.825	31.633	31.825	1.00 16.80
		-						
MOTA	1062	CD2	LEU A	194	10.585	30.044	31.014	1.00 16.32
MOTA	1063	N	GLU A	195	9.025	34.150	28.095	1.00 18.44
MOTA	1064	CA	GLU A	195	9.949	35.029	27.369	1.00 18.80
MOTA	1065	С	GLU A		11.415	34.777	27.733	1.00 19.02
ATOM	1066	0	GLU A	195	11.791	34.754	28.953	1.00 17.72
ATOM	1067	CB	GLU A	195	9.575	36.485	27.644	1.00 20.83
			GLU A		10.514	37.512	27.047	1.00 23.03
MOTA	1068	CG						
ATOM	1069	CD	GLU F	195	9.989	38.926	27.204	1.00 24.10
ATOM	1070	OE1	GLU A	195	9.211	39.373	26.337	1.00 25.77
ATOM	1071	OE2	GLU A		10.343	39.585	28.203	1.00 24.06
MOTA	1072	N	PRO P	196	12.272	34.559	26.714	1.00 18.43
MOTA	1073	CA	PRO F	196	13.702	34.311	26.935	1.00 18.17
ATOM	1074	С	PRO A		14.385	35.571	27.447	1.00 16.90
ATOM	1075	0	PRO A		13.845	36.715	27.297	1.00 17.67
MOTA	1076	CB	PRO F	196	14.210	33.914	25.546	1.00 17.79
ATOM	1077	CG	PRO F	196	12.992	33.305	24.892	1.00 19.11
ATOM	1078	CD	PRO F		11.911	34.287	25.310	1.00 18.58
MOTA	1079	N	PHE A	197	15.558	35.405	28.039	1.00 15.80
MOTA	1080	CA	PHE A	197	16.290	36.550	28.574	1.00 14.47
ATOM	1081	C	PHE A		16.597	37.663	27.576	1.00 16.31
MOTA	1082	0	PHE P		16.392	38.873	27.894	1.00 14.87
ATOM	1083	CB	PHE A	197	17.595	36.093	29.217	1.00 12.99
MOTA	1084	CG	PHE A		18.472	37.227	29.652	1.00 13.09
ATOM	1085	CD1	PHE A		19.376	37.806	28.767	1.00 12.33
ATOM	1086	CD2	PHE P	197	18.347	37.766	30.926	1.00 14.29
ATOM	1087	CE1	PHE A	197	20.139	38.907	29.143	1.00 12.22
ATOM	1088	CE2	PHE A		19.108	38.873	31.310	1.00 14.64
MOTA	1089	CZ	PHE A	197	20.002	39.441	30.415	1.00 13.26
MOTA	1090	N	PHE A	198	17.089	37.319	26.390	1.00 16.71
MOTA	1091	CA	PHE A		17.427	38.384	25.431	1.00 17.60
MOTA	1092	С	PHE A		16.212	39.192	25.001	1.00 17.52
MOTA	1093	0	PHE A	198	16.317	40.434	24.774	1.00 16.03
MOTA	1094	CB	PHE A	1.98	18.133	37.829	24.196	1.00 17.77
	1095		PHE A				23.549	1.00 17.92
MOTA		CG			19.051	38.826		
MOTA	1096	CD1	PHE A	. 198	20.310	39.075	24.087	1.00 18.66
MOTA	1097	CD2	PHE A	198	18.633	39.569	22.455	1.00 16.90
MOTA	1098		PHE A		21.139	40.053	23.546	1.00 18.55
MOTA	1099	CE2			19.454	40.551	21.904	1.00 17.96
ATOM	1100	CZ	PHE A	198	20.708	40.795	22.451	1.00 18.52
MOTA	1101	N	ASP A		15.066	38.530	24.879	1.00 17.52
MOTA	1102	CA	ASP A		13.819	39.225	24.491	1.00 19.54
ATOM	1103	С	ASP A	. 199	13.464	40.261	25.561	1.00 18.83
MOTA	1104	0	ASP A	199	13.134	41.444	25.233	1.00 20.48
ATOM	1105	СВ	ASP A		12.685	38.210	24.338	1.00 21.95
MOTA	1106	CG	ASP A		12.868	37.312	23.126	1.00 24.77
ATOM	1107	OD1	ASP A	199	12.408	37.687	22.028	1.00 27.27
ATOM	1108		ASP A		13.481	36.234	23.261	1.00 27.11
ATOM								1.00 17.89
	1109	N	SER A		13.530	39.858	26.829	
MOTA	1110	CA	SER A		13.223	40.784	27.947	1.00 16.17
MOTA	1111	С	SER A	200	14.211	41.943	27.915	1.00 16.77
MOTA	1112	0	SER A		13.823	43.140	28.072	1.00 17.20
		-	~~ F		13.023	43.14U	20.072	

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MOTA	1113	CB	SER	Α	200	13.336	40.062	29.292	1.00 14.55
ATOM	1114	OG	SER	Α	200	12.386	39.017	29.400	1.00 14.16
	1115	N	LEU			15.481	41.617	27.711	1.00 16.47
ATOM									
ATOM	1116	CA	LEU	A	201	16.553	42.638	27.654	1.00 18.93
MOTA	1117	С	LEU	Α	201	16.237	43.684	26.586	1.00 18.88
ATOM	1118	0	LEU	Δ	201	16.274	44.917	26.852	1.00 18.26
MOTA	1119	CB	LEU			17.884	41.953	27.337	1.00 18.68
MOTA	1120	CG	LEU	Α	201	19.244	42.637	27.523	1.00 20.59
MOTA	1121	CD1	LEU	A	201	19.973	42.616	26.194	1.00 20.98
						19.100	44.053	28.045	1.00 20.13
ATOM	1122		LEU						
MOTA	1123	N	VAL	A	202	15.919	43.222	25.383	1.00 20.38
ATOM	1124	CA	VAL	Α	202	15.600	44.130	24.264	1.00 20.23
	1125	C	VAL			14.335	44.938	24.532	1.00 23.13
MOTA									
MOTA	1126	0	VAL	Α	202	14.284	46.175	24.255	1.00 23.36
ATOM	1127	CB	VAL	Α	202	15.433	43.337	22.948	1.00 19.84
ATOM	1128	CG1	VAL	Δ	202	14.830	44.228	21.855	1.00 17.60
								22.502	1.00 16.36
MOTA	1129		VAL			16.792	42.804		
MOTA	1130	N	LYS	Α	203	13.315	44.285	25.074	1.00 24.15
MOTA	1131	CA	LYS	Α	203	12.050	44.985	25.360	1.00 27.77
	1132	C	LYS			12.178	46.049	26.452	1.00 27.47
MOTA									
MOTA	1133	0	LYS	Α	203	11.753	47.223	26.252	1.00 26.63
MOTA	1134	CB	LYS	Α	203	10.970	43.973	25.746	1.00 29.55
ATOM	1135	CG	LYS	Δ	203	9.609	44.594	26.008	1.00 34.08
MOTA	1136	CD	LYS			8.497	43.798	25.335	1.00 36.82
MOTA	1137	CE	LYS	Α	203	8.504	42.342	25.774	1.00 38.97
ATOM	1138	NZ	LYS	Α	203	7.512	41.533	25.012	1.00 40.86
-	1139				204	12.771	45.687	27.585	1.00 26.46
MOTA		N							
MOTA	1140	CA			204	12.910	46.632	28.721	1.00 26.94
MOTA	1141	С	GLN	Α	204	14.125	47.542	28.614	1.00 28.51
ATOM	1142	0	GLN			14.479	48.264	29.600	1.00 30.36
ATOM	1143	CB	GLN			13.007	45.848	30.032	1.00 24.17
MOTA	1144	CG	GLN	А	204	11.980	44.739	30.170	1.00 20.78
ATOM	1145	CD	GLN	А	204	12.270	43.821	31.342	1.00 20.14
	1146		GLN			11.725	42.676	31.420	1.00 19.72
MOTA									
MOTA	1147	NE2	GLN	A	204	13.107	44.279	32.265	1.00 16.56
ATOM	1148	N	THR	Α	205	14.762	47.568	27.453	1.00 28.58
ATOM	1149	CA	THR	Α	205	15.979	48.375	27.306	1.00 29.06
								25.885	1.00 30.58
MOTA	1150	С			205	16.186	48.905		
MOTA	1151	0	THR	А	205	15.427	48.525	24.940	1.00 30.23
ATOM	1152	CB	THR	Α	205	17.175	47.501	27.772	1.00 29.85
ATOM	1153	OG1				17.572	47.899	29.088	1.00 29.62
MOTA	1154	CG2	THR			18.328	47.576	26.823	1.00 29.03
MOTA	1155	N	HIS	Α	206	17.175	49.784	25.711	1.00 31.92
ATOM	1156	CA	HTS	A	206	17.488	50.350	24.372	1.00 33.38
		C	HIS			18.548	49.530	23.637	1.00 32.31
ATOM	1157								
MOTA	1158	0	HIS			18.905	49.845	22.460	1.00 31.08
MOTA	1159	CB	HIS	Α	206	17.975	51.799	24.487	1.00 36.39
MOTA	1160	CG	HIS			16.898	52.773	24.848	1.00 39.92
								24.177	1.00 40.95
MOTA	1161		HIS			15.696	52.836		
ATOM	1162	CD2	HIS	Α	206	16.849	53.736	25.800	1.00 40.35
MOTA	1163	CE1	HIS	Α	206	14.951	53.794	24.699	1.00 41.58
ATOM	1164		HIS			15.627	54.356	25.685	1.00 41.65
ATOM	1165	N	VAL			19.075	48.501	24.291	1.00 29.55
MOTA	1166	CA	VAL	Α	207	20.097	47.639	23.651	1.00 28.49
ATOM	1167	С	VAL			19.511	47.083	22.354	1.00 26.27
ATOM			VAL				46.441	22.358	1.00 26.26
	1168	0				18.415			
ATOM	1169	СВ	VAL			20.498	46.462	24.572	1.00 28.77
MOTA	1170	CG1	VAL	Α	207	21.399	45.491	23.825	1.00 29.45
ATOM	1171		VAL			21.219	46.987	25.805	1.00 28.52
	1172				208	20.192	47.311	21.220	1.00 24.42
MOTA		N							
MOTA	1173	CA			208	19.683	46.804	19.944	1.00 23.82
MOTA	1174	С	PRO	Α	208	19.547	45.284	19.914	1.00 22.81

MOTA	1175	0	PRO	А	208	20.290	44.545	20.630	1.00 21.12
ATOM	1176	CB	PRO	Α	208	20.689	47.343	18.926	1.00 24.65
ATOM	1177	CG			208	21.927	47.510	19.711	1.00 25.77
MOTA	1178	CD	PRO			21.441	48.062	21.025	1.00 24.39
ATOM	1179	N	ASN	Α	209	18.605	44.806	19.109	1.00 21.59
MOTA	1180	CA	ASN	Α	209	18.322	43.362	18.995	1.00 20.43
ATOM	1181	C	ASN			19.390	42.599	18.222	1.00 20.52
						19.190	42.217	17.026	1.00 21.39
ATOM	1182	0	ASN						
MOTA	1183	CB	ASN			16.957	43.159	18.340	1.00 18.52
MOTA	1184	CG	ASN	Α	209	16.501	41.728	18.402	1.00 18.12
ATOM	1185	OD1	ASN	Α	209	16.968	40.948	19.281	1.00 18.32
	1186		ASN			15.594	41.348	17.513	1.00 15.63
ATOM							42.346	18.883	1.00 19.53
ATOM	1187	N	LEU			20.514			
MOTA	1188	CA	LEU	Α	210	21.631	41.634	18.243	1.00 19.83
ATOM	1189	С	LEU	Α	210	22.765	41.421	19.226	1.00 19.02
ATOM	1190	0	LEU	Α	210	22.958	42.238	20.176	1.00 18.52
ATOM	1191	СВ	LEU			22.120	42.451	17.035	1.00 21.93
ATOM	1192	CG	LEU			23.534	42.305	16.456	1.00 22.75
MOTA	1193		LEU			23.612	43.009	15.102	1.00 23.20
ATOM	1194	CD2	LEU	Α	210	24.548	42.910	17.409	1.00 24.60
MOTA	1195	N	PHE	Α	211	23.509	40.334	19.044	1.00 16.48
ATOM	1196	CA	PHE			24.671	40.055	19.909	1.00 16.70
MOTA	1197	С	PHE			25.722	39.310	19.095	1.00 16.08
MOTA	1198	0	PHE	Α	211	25.392	38.653	18.063	1.00 17.22
ATOM	1199	CB	PHE	Α	211	24.251	39.280	21.173	1.00 14.67
ATOM	1200	CG	PHE	Α	211	23.813	37.863	20.924	1.00 16.01
ATOM	1201		PHE			24.748	36.837	20.835	1.00 14.91
		-							1.00 14.62
ATOM	1202	-	PHE			22.465	37.546	20.824	
MOTA	1203	CE1	PHE	Α	211	24.344	35.515	20.653	1.00 15.05
ATOM	1204	CE2	PHE	Α	211	22.054	36.224	20.641	1.00 15.47
ATOM	1205	$\mathbf{C}\mathbf{Z}$	PHE	Α	211	22.996	35.207	20.558	1.00 12.73
MOTA	1206	N			212	26.977	39.424	19.520	1.00 17.19
ATOM	1207	CA	SER			28.126	38.803	18.818	1.00 16.98
ATOM	1208	С	SER	A	212	28.894	37.862	19.725	1.00 16.10
ATOM	1209	0	SER	Α	212	29.036	38.122	20.955	1.00 14.22
MOTA	1210	CB	SER	Α	212	29.094	39.888	18.349	1.00 16.89
ATOM	1211	OG	SER			28.431	40.869	17.593	1.00 26.70
MOTA	1212	N	LEU			29.430	36.797	19.144	1.00 14.76
MOTA	1213	CA	LEU			30.194	35.819	19.930	1.00 14.81
MOTA	1214	C	LEU	Α	213	31.563	35.509	19.352	1.00 14.32
MOTA	1215	0	LEU	Α	213	31.702	35.162	18.137	1.00 12.74
ATOM	1216	CB	LEU			29.394	34.522	20.060	1.00 15.67
									1.00 18.95
MOTA	1217	CG	LEU			28.735	34.210	21.408	
MOTA	1218		LEU			28.196	35.475	22.050	1.00 18.65
ATOM	1219	CD2	LEU			27.627	33.185	21.192	1.00 16.46
ATOM	1220	N	GLN	Α	214	32.581	35.656	20.191	1.00 14.19
MOTA	1221	CA			214	33.954	35.324	19.797	1.00 15.89
			GLN			34.407		20.778	1.00 15.04
MOTA	1222	C					34.258		
MOTA	1223	0	GLN			34.848	34.582	21.917	1.00 16.01
MOTA	1224	CB	GLN	Α	214	34.903	36.523	19.914	1.00 17.92
MOTA	1225	CG	GLN	Α	214	36.290	36.231	19.341	1.00 20.63
ATOM	1226	CD	GLN			37.397	37.099	19.932	1.00 23.22
								19.273	1.00 24.79
ATOM	1227		GLN			38.459	37.332		
ATOM	1228		GLN			37.199	37.571	21.156	1.00 24.53
MOTA	1229	N	LEU			34.284	32.997	20.390	1.00 14.37
MOTA	1230	CA	LEU	Α	215	34.729	31.890.	21.262	1.00 13.74
ATOM	1231	C	LEU			36.193	31.625	20.925	1.00 14.40
			LEU					19.737	1.00 14.39
MOTA	1232	0				36.541	31.357		
ATOM	1233	CB	LEU			33.872	30.644	21.005	1.00 13.94
MOTA	1234	CG	LEU	Α	215	32.636	30.429	21.893	1.00 14.78
MOTA	1235	CD1	LEU	Α	215	31.900	31.734	22.143	1.00 13.31
MOTA	1236		LEU			31.723	29.407	21.240	1.00 12.97
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MOTA	1237	N	CYS	Α	216	37.066	31.706	21.922	1.00 14.83
MOTA	1238	CA	CYS	Α	216	38.504	31.486	21.682	1.00 16.37
						39.066	30.196	22.263	1.00 17.20
MOTA	1239	С	CYS						
MOTA	1240	0	CYS	Α	216	39.174	30.046	23.519	1.00 16.79
ATOM	1241	CB	CYS	A	216	39.314	32.668	22.227	1.00 19.03
MOTA	1242	SG	CYS			38.852	34.278	21.505	1.00 23.75
MOTA	1243	N	GLY	A	217	39.415	29.257	21.387	1.00 15.43
MOTA	1244	CA	GLY	Δ	217	40.018	28.021	21.843	1.00 16.40
ATOM	1245	С	GLY			41.483	28.371	22.064	1.00 17.87
ATOM	1246	0	GLY	Α	217	42.057	29.204	21.303	1.00 17.53
ATOM	1247	N	ALA	Δ	218	42.119	27.785	23.069	1.00 17.79
ATOM	1248	CA	ALA			43.539	28.108	23.349	1.00 16.33
ATOM	1249	C	ALA	A	218	44.486	27.408	22.379	1.00 17.71
MOTA	1250	0	ALA	Δ	218	45.602	27.927	22.069	1.00 16.46
								24.779	1.00 14.95
MOTA	1251	CB	ALA			43.884	27.731		
ATOM	1252	N	GLY	А	219	44.073	26.245	21.890	1.00 16.19
ATOM	1253	CA	GLY	Α	219	44.909	25.505	20.970	1.00 17.57
	1254	C	GLY			45.696	24.439	21.703	1.00 17.52
MOTA									
ATOM	1255	0	GLY	Α	219	46.490	23.675	21.076	1.00 16.29
ATOM	1256	N	PHE	Α	220	45.502	24.375	23.018	1.00 17.13
	1257	CA	PHE			46.190	23.381	23.873	1.00 18.29
ATOM									
ATOM	1258	С	PHE	A	220	45.381	23.185	25.153	1.00 19.24
ATOM	1259	0	PHE	Α	220	44.477	24.012	25.475	1.00 19.69
ATOM	1260	CB	PHE			47.616	23.854	24.187	1.00 18.72
MOTA	1261	CG	PHE	A	220	47.689	25.253	24.731	1.00 20.07
MOTA	1262	CD1	PHE	Α	220	47.448	25.507	26.077	1.00 20.91
MOTA	1263	CD2	PHE	7	220	47.984	26.320	23.890	1.00 19.91
ATOM	1264	CEI	PHE	A	220	47.505	26.809	26.576	1.00 21.79
ATOM	1265	CE2	PHE	A	220	48.043	27.620	24.374	1.00 20.35
ATOM	1266	CZ	PHE			47.802	27.866	25.721	1.00 21.77
ATOM	1267	N	PRO		_	45.659	22.110	25.907	1.00 20.17
MOTA	1268	CA	PRO	Α	221	44.922	21.846	27.147	1.00 21.27
MOTA	1269	С	PRO	A	221	45.014	22.959	28.180	1.00 23.04
									1.00 23.99
MOTA	1270	0	PRO			46.065	23.666	28.292	
MOTA	1271	CB	PRO	А	221	45.545	20.543	27.648	1.00 20.22
ATOM	1272	CG	PRO	А	221	45.946	19.855	26.390	1.00 20.63
MOTA	1273	CD	PRO			46.571	20.994	25.602	1.00 20.45
ATOM	1274	N	LEU	Α	222	43.934	23.132	28.933	1.00 25.72
MOTA	1275	CA	LEU	Α	222	43.873	24.158	29.991	1.00 28.32
ATOM	1276	C	LEU			43.425	23.516	31.291	1.00 30.88
MOTA	1277	0	LEU	А	222	42.248	23.042	31.403	1.00 31.71
MOTA	1278	CB	LEU	Α	222	42.880	25.261	29.620	1.00 27.52
ATOM	1279	CG	LEU	Δ	222	43.264	26.233	28.506	1.00 27.30
MOTA	1280		LEU			42.040	27.042	28.096	
MOTA	1281	CD2	LEU	Α	222	44.382	27.143	28.983	1.00 27.13
MOTA	1282	N	ASN			44.320	23.470	32.273	1.00 34.15
			ASN			43.959	22.893	33.583	1.00 37.64
MOTA	1283	CA							
MOTA	1284	С	ASN	Α	223	43.014	23.882	34.254	1.00 38.54
ATOM	1285	0	ASN	Α	223	42.864	25.056	33.785	1.00 36.72
			ASN				22.663	34.457	1.00 38.54
MOTA	1286	CB				45.204			
MOTA	1287	CG	ASN	A	223	45.905	23.952	34.839	1.00 39.09
MOTA	1288	OD1	ASN	Α	223	45.268	24.903	35.375	1.00 41.39
ATOM	1289		ASN				24.013	34.595	1.00 40.09
ATOM	1290	N	GLN			42.380	23.444	35.335	1.00 41.79
ATOM	1291	CA	GLN	Α	224	41.415	24.278	36.073	1.00 43.58
ATOM					224	41.898	25.708	36.359	1.00 42.52
	1292	C			~~ =	31.030	23.700		44.56
	1292	C			224	41 170	26 725	26 126	1 00 40 75
MOTA	1293	0	GLN	A		41.138	26.705	36.126	1.00 42.75
ATOM ATOM				A		41.138 41.021	26.705 23.572	36.126 37.378	1.00 42.75 1.00 46.22
MOTA	1293 1294	O CB	GLN GLN	A A	224	41.021	23.572	37.378	1.00 46.22
MOTA MOTA	1293 1294 1295	O CB CG	GLN GLN	A A A	224 224	41.021 39.629	23.572 23.956	37.378 37.827	1.00 46.22 1.00 49.86
MOTA MOTA MOTA	1293 1294 1295 1296	O CB CG CD	GLN GLN GLN GLN	A A A	224 224 224	41.021 39.629 39.085	23.572 23.956 23.160	37.378 37.827 38.990	1.00 46.22 1.00 49.86 1.00 51.40
MOTA MOTA	1293 1294 1295	O CB CG CD	GLN GLN	A A A	224 224 224	41.021 39.629	23.572 23.956	37.378 37.827 38.990 39.443	1.00 46.22 1.00 49.86
MOTA MOTA MOTA	1293 1294 1295 1296	O CB CG CD OE1	GLN GLN GLN GLN	A A A A	224 224 224 224	41.021 39.629 39.085	23.572 23.956 23.160	37.378 37.827 38.990	1.00 46.22 1.00 49.86 1.00 51.40

				_			05 050	26 021	1 00 40 07
MOTA	1299	N	SER			43.133	25.852	36.831	1.00 40.27
MOTA	1300	CA	SER	Α	225	43.669	27.200	37.138	1.00 39.30
			SER			43.989	28.028	35.893	1.00 36.57
MOTA	1301	С							
MOTA	1302	0	SER	Α	225	43.920	29.292	35.930	1.00 36.27
MOTA	1303	CB	SER	Δ	225	44.917	27.094	38.027	1.00 40.27
MOTA	1304	OG	SER	Α	225	45.974	26.411	37.376	1.00 42.21
ATOM	1305	N	GLU	Α	226	44.339	27.364	34.796	1.00 34.29
			GLU			44.654	28.083	33.542	1.00 32.79
MOTA	1306	CA							
MOTA	1307	С	GLU	А	226	43.375	28.651	32.954	1.00 31.17
MOTA	1308	0	GLU	Δ	226	43.354	29.815	32.454	1.00 29.09
		_							
MOTA	1309	СВ	GLU			45.307	27.144	32.526	1.00 33.69
ATOM	1310	CG	GLU	Α	226	46.708	26.696	32.902	1.00 36.40
	1311	CD	GLU			47.251	25.619	31.972	1.00 37.70
MOTA									
MOTA	1312		GLU			46.585	24.567	31.830	1.00 37.54
MOTA	1313	OE2	GLU	Α	226	48.340	25.823	31.389	1.00 37.14
	1314		VAL			42.305	27.867	33.007	1.00 29.89
MOTA		N						•	
MOTA	1315	CA	VAL	Α	227	41.013	28.312	32.458	1.00 30.15
MOTA	1316	С	VAL	A	227	40.512	29.547	33.203	1.00 29.84
								32.582	1.00 30.30
MOTA	1317	0	VAL			39.922	30.484		
ATOM	1318	CB	VAL	Α	227	39.940	27.210	32.558	1.00 30.93
MOTA	1319	CG1	VAL	2	227	38.800	27.538	31.637	1.00 32.67
ATOM	1320	ÇG2	VAL	A	227	40.516	25.867	32.183	1.00 32.31
MOTA	1321	N	LEU	Α	228	40.731	29.581	34.513	1.00 28.88
	1322	CA.	LEU			40.292	30.726	35.336	1.00 27.31
ATOM									
MOTA	1323	С	LEU	Α	228	41.059	31.992	34.975	1.00 27.59
MOTA	1324	0	LEU	Α	228	40.491	33.129	35.020	1.00 27.84
			LEU			40.496	30.420	36.819	1.00 27.50
MOTA	1325	CB							
ATOM	1326	CG	LEU	Α	228	39.700	29.259	37.419	1.00 29.32
MOTA	1327	CD1	LEU	Α	228	40.129	29.053	38.867	1.00 28.16
			LEU			38.205	29.549	37.339	1.00 28.58
MOTA	1328								
ATOM	1329	N	ALA	Α	229	42.327	31.835	34.610	1.00 27.12
MOTA	1330	CA	ALA	Α	229	43.176	32.998	34.257	1.00 27.64
	1331	С	ALA			43.134	33.347	32.776	1.00 27.65
ATOM									
MOTA	1332	0	ALA	Α	229	43.460	34.504	32.375	1.00 29.94
ATOM	1333	CB	ALA	А	229	44.617	32.736	34.682	1.00 27.52
			SER			42.736	32.393	31.947	1.00 26.68
ATOM	1334	И							
ATOM	1335	CA	SER	Α	230 ·	42.692	32.635	30.498	1.00 26.33
MOTA	1336	С	SER	Α	230	41.438	33.360	30.032	1.00 26.22
								30.695	1.00 25.70
MOTA	1337	0			230	40.356	33.302		
MOTA	1338	CB	SER	A	230	42.815	31.310	29.746	1.00 26.07
ATOM	1339	OG	SER	Δ	230	42.759	31.519	28.344	1.00 26.54
MOTA	1340	N	VAL			41.562	34.056	28.909	1.00 25.03
ATOM	1341	CA	VAL	Α	231	40.415	34.764	28.320	1.00 24.89
ATOM	1342	С	VAL	Δ	231	39.785	33.776	27.346	1.00 24.75
		-					33.310		1.00 25.97
ATOM	1343	0	VAL			40.453		26.371	
ATOM	1344	CB	VAL	Α	231	40.859	36.043	27.568	1.00 24.38
ATOM	1345	CG1	VAL	Δ	231	39.729	36.554	26.678	1.00 22.98
									1.00 23.20
ATOM	1346	CGZ	VAL			41.244	37.119	28.577	
MOTA	1347	N	GLY	Α	232	38.526	33.433	27.588	1.00 23.26
ATOM	1348	CA	GLY			37.846	32.481	26.729	1.00 22.77
MOTA	1349	С	GLY	Α	232	37.125	33.081	25.538	1.00 21.57
MOTA	1350	0	GLY	Α	232	36.590	32.324	24.666	1.00 20.69
	1351	N	GLY			37.078	34.408	25.468	1.00 19.21
ATOM									
MOTA	1352	CA	GLY	A	233	36.410	35.050	24.353	1.00 17.96
MOTA	1353	С	GLY	Α	233	35.599	36.275	24.731	1.00 18.25
			GLY			35.778	36.866	25.851	1.00 15.19
ATOM	1354	0							
MOTA	1355	N	SER	Α	234	34.708	36.677	23.828	1.00 16.58
MOTA	1356	CA	SER	Α	234	33.864	37.864	24.053	1.00 16.83
ATOM	1357	C			234	32.423	37.667	23.599	1.00 17.82
ATOM	1358	0			234	32.134	36.995	22.552	1.00 17.90
MOTA	1359	CB	SER	Α	234	34.426	39.072	23.291	1.00 16.36
		OG			234		39.253	23.508	1.00 18.23
MOTA	1360	OG	المتار	•	233	35.816	33.233	23.300	1.00 10.23

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MOTA	1361	N	MET A	235	31.506	38.227	24.372	1.00 18.00
MOTA	1362	CA	MET A	235	30.091	38.201	24.010	1.00 17.58
ATOM	1363	С	MET A	235	29.732	39.677	23.996	1.00 18.27
ATOM	1364	0	MET A	235	29.594	40.322	25.087	1.00 19.03
MOTA	1365	СВ	MET A		29.232	37.475	25.046	1.00 16.91
ATOM	1366	CG	MET A		27.759	37.455	24.634	1.00 17.60
			MET A		26.597	36.751	25.819	1.00 20.56
ATOM	1367	SD						
ATOM	1368	CE	MET A		25.105	36.803	24.857	1.00 21.69
MOTA	1369	N	ILE A		29.629	40.248	22.801	1.00 19.70
MOTA	1370	CA	ILE A		29.271	41.669	22.674	1.00 19.40
MOTA	1371	С	ILE A		27.764	41.758	22.522	1.00 20.06
MOTA	1372	0	ILE A	236	27.175	41.365	21.467	1.00 16.87
ATOM	1373	CB	ILE A	236	29.985	42.341	21.470	1.00 21.41
MOTA	1374	CG1	ILE A	236	31.452	42.625	21.821	1.00 22.57
MOTA	1375	CG2	ILE A	236	29.329	43.672	21.149	1.00 21.72
MOTA	1376	CD1	ILE A	236	32.243	41.426	22.228	1.00 25.65
MOTA	1377	N	ILE A	237	27.122	42.246	23.575	1.00 20.16
ATOM	1378	CA	ILE A		25.663	42.382	23.599	1.00 21.01
ATOM	1379	C	ILE A		25.215	43.710	22.996	1.00 22.16
ATOM	1380	ō	ILE A		25.620	44.812	23.472	1.00 22.96
ATOM	1381	СВ	ILE A		25.153	42.241	25.050	1.00 21.36
ATOM	1382	CG1			25.346	40.791	25.498	1.00 22.29
	1382	CG2	ILE A		23.694	42.660	25.156	1.00 20.45
ATOM					25.002	40.529	26.939	1.00 20.43
ATOM	1384	CD1	ILE A					
ATOM	1385	N	GLY A		24.404	43.626	21.946	1.00 23.30
ATOM	1386	CA	GLY A		23.903	44.820	21.288	1.00 25.11
MOTA	1387	C	GLY A		24.821	45.437	20.244	1.00 26.35
ATOM	1388	0	GLY A		24.644	46.640	19.874	1.00 27.08
MOTA	1389	N	GLY A		25.792	44.681	19.743	1.00 25.50
MOTA	1390	CA	GLY A		26.679	45.251	18.747	1.00 24.81
ATOM	1391	С	GLY A	239	27.807	44.371	18.242	1.00 26.38
MOTA	1392	0	GLY A	239	27.942	43.167	18.632	1.00 23.61
MOTA	1393	N	ILE A	240	28.632	44.960	17.383	1.00 26.33
ATOM	1394	CA	ILE A	240	29.780	44.273	16.758	1.00 25.87
MOTA	1395	С	ILE A	240	31.067	45.033	17.055	1.00 26.95
ATOM	1396	0	ILE A	240	31.121	46.287	16.882	1.00 28.86
ATOM	1397	СВ	ILE A	240	29.607	44.226	15.226	1.00 25.88
ATOM	1398	CG1	ILE A	240	28.298	43.519	14.871	1.00 25.12
ATOM	1399	CG2	ILE A		30.806	43.541	14.581	1.00 26.56
ATOM	1400	CD1	ILE A		27.939	43.599	13.396	1.00 24.59
ATOM	1401	N	ASP A		32.100	44.323	17.498	1.00 25.24
ATOM	1402	CA	ASP A		33.395	44.973	17.781	1.00 25.13
ATOM	1403	C	ASP A		34.383	44.548	16.698	1.00 26.31
ATOM	1404	ō	ASP A		34.676		16.536	
MOTA	1405	СВ	ASP A		33.922	44.561	19.153	1.00 24.85
ATOM	1406	CG	ASP A		35.171	45.325	19.541	1.00 24.81
						46.032	20.567	
ATOM	1407		ASP A		35.144			1.00 27.86
ATOM	1408		ASP A			45.226	18.817	1.00 25.69
MOTA	1409	И	HIS A			45.517	15.960	1.00 26.86
MOTA	1410	CA	HIS A		35.853	45.222	14.852	1.00 27.45
MOTA	1411	C	HIS A		37.197	44.613	15.221	1.00 25.41
MOTA	1412	0	HIS A		37.871	43.998	14.347	1.00 23.94
MOTA	1413	СВ	HIS A		36.085	46.481	14.013	1.00 32.38
ATOM	1414	CG	HIS A		34.858	46.957	13.304	1.00 37.46
MOTA	1415	ND1	HIS A	242	33.822	47.591	13.956	1.00 39.65
MOTA	1416	CD2	HIS A	242	34.472	46.837	12.011	1.00 39.29
ATOM	1417	CE1	HIS A	242	32.850	47.840	13.096	1.00 40.56
MOTA	1418	NE2	HIS A	242	33.219	47.392	11.909	1.00 40.36
MOTA	1419	N	SER A	243		44.751	16.471	1.00 22.23
ATOM	1420	CA	SER A			44.184	16.877	1.00 22.06
ATOM	1421	С	SER A			42.667	17.011	1.00 20.51
MOTA	1422	0	SER A	243		41.986	17.130	1.00 23.23

MOTA	1423	CB	SER A	. 243	39.368	44.785	18.211	1.00 22.47
MOTA	1424	OG	SER A	243	38.515	44.386	19.274	1.00 23.32
			LEU A		37.635	42.115	16.979	1.00 20.52
MOTA	1425	N	_					
MOTA	1426	CA	LEU A		37.454	40.649	17.145	1.00 18.32
ATOM	1427	С	LEU A	. 244	37.535	39.844	15.860	1.00 18.66
ATOM	1428	0	LEU A	244	37.482	38.576	15.892	1.00 18.25
ATOM	1429	CB	LEU A		36.120	40.368	17.843	1.00 18.01
•								
MOTA	1430	CG	LEU A		35.998	41.054	19.206	1.00 17.93
ATOM	1431	CD1	LEU A	. 244	34.689	40.666	19.885	1.00 17.04
ATOM	1432	CD2	LEU A	244	37.189	40.661	20.063	1.00 19.23
MOTA	1433	N	TYR A	245	37.666	40.522	14.729	1.00 18.73
ATOM	1434	CA	TYR A		37.756	39.795	13.459	1.00 19.72
MOTA	1435	С	TYR A		38.536	40.545	12.398	1.00 20.55
ATOM	1436	0	TYR A		38.819	41.771	12.542	1.00 21.10
ATOM	1437	CB	TYR A	. 245	36.357	39.494	12.924	1.00 19.56
ATOM	1438	CG	TYR A	245	35.606	40.708	12.421	1.00 20.40
ATOM	1439	CD1	TYR A	245	34.977	41.586	13.302	1.00 20.11
ATOM	1440	CD2	TYR A		35.512	40.966	11.055	1.00 20.70
ATOM	1441	CE1	TYR A		34.265	42.689	12.834	1.00 21.90
MOTA	1442	CE2	TYR A	. 245	34.809	42.060	10.573	1.00 22.10
ATOM	1443	CZ	TYR A	. 245	34.184	42.919	11.466	1.00 23.05
ATOM	1444	ОН	TYR A	245	33.476	43.993	10.979	1.00 22.53
ATOM	1445	N	THR A		38.902	39.829	11.340	1.00 20.48
								1.00 19.46
MOTA	1446	CA	THR A		39.621	40.429	10.195	
MOTA	1447	С	THR A	. 246	38.811	40.054	8.964	1.00 19.29
MOTA	1448	0	THR A	. 246	37.999	39.085	9.000	1.00 16.84
MOTA	1449	CB	THR A	246	41.049	39.865	10.031	1.00 19.69
ATOM	1450	OG1			40.997	38.434	9.953	1.00 20.05
	1451	CG2	THR A		41.929	40.294	11.194	1.00 19.01
MOTA								
MOTA	1452	N	GLY A		38.996	40.793	7.879	1.00 19.48
ATOM	1453	CA	GLY A	. 247	38.259	40.490	6.668	1.00 19.61
MOTA	1454	С	GLY A	247	36.812	40.927	6.747	1.00 20.26
MOTA	1455	0	GLY A	247	36.412	41.712	7.660	1.00 21.64
ATOM	1456	N	SER A		36.006	40.437	5.816	1.00 21.23
MOTA	1457	CA	SER A		34.580	40.806	5.765	1.00 23.54
							6.484	1.00 23.00
ATOM	1458	C	SER A		33.649	39.836		
ATOM	1459	0	SER A		33.978	38.625	6.684	1.00 21.96
MOTA	1460	CB	SER A		34.135	40.936	4.304	1.00 24.06
ATOM	1461	OG	SER A	248	34.814	41.999	3.656	1.00 28.27
MOTA	1462	N	LEU A		32.494	40.355	6.881	1.00 23.33
MOTA	1463	CA	LEU A		31.453	39.551	7.550	1.00 23.71
			LEU A			39.103	6.468	1.00 23.26
MOTA	1464	C			30.478			
MOTA	1465	0	LEU A		29.913	39.958	5.721	1.00 24.66
MOTA	1466	CB	LEU A	249	30.687	40.392	8.57 <i>6</i>	1.00 22.83
ATOM	1467	CG	LEU A	249	31.234	40.585	9.992	1.00 23.68
ATOM	1468	CD1	LEU A	249	30.483	41.728	10.659	1.00 23.07
ATOM	1469		LEU A		31.077	39.299	10.802	1.00 22.16
	1470		TRP A		30.285	37.797	6.335	1.00 21.28
MOTA		N						
MOTA	1471	CA	TRP A		29.328	37.282	5.348	1.00 18.03
MOTA	1472	C	TRP A	250	28.115	36.810	6.115	1.00 18.51
MOTA	1473	0	TRP A	250	28.242	36.079	7.153	1.00 18.65
ATOM	1474	CB	TRP A	250	29.925	36.128	4.550	1.00 19.15
ATOM	1475	CG	TRP A		30.759	36.597	3.411	1.00 19.10
								1.00 18.51
MOTA	1476	CD1	TRP A		32.061	36.998	3.456	
ATOM	1477	CD2	TRP A		30.328	36.777	2.058	1.00 18.74
MOTA	1478	NE1	TRP A	250	32.470	37.418	2.214	1.00 18.41
ATOM	1479	CE2	TRP A		31.425	37.294	1.336	1.00 18.71
MOTA	1480	CE3	TRP A		29.118	36.554	1.386	1.00 19.61
ATOM	1481	CZ2	TRP A		31.352	37.594	-0.029	1.00 18.57
							0.026	1.00 20.92
ATOM	1482	CZ3	TRP A		29.043	36.853		
MOTA	1483	CH2	TRP A		30.158	37.369	-0.666	1.00 17.98
MOTA	1484	N	TYR A	251 ·	26.939	37.203	5.644	1.00 17.22
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ATOM	1485	CA			251	25.699	36.825	6.328	1.00 16.85
ATOM	1486	С	TYR	A	251	24.875	35.751	5.642	1.00 16.82
MOTA	1487.	Ō			251	24.668	35.782		
								4.397	1.00 17.05
ATOM	1488	CB	TYR	A	251	24.814	38.059	6.536	1.00 17.46
ATOM	1489	CG	TYR	Α	251	25.389	39.070	7.493	1.00 17.27
ATOM	1490	CD1			251	26.265	40.065	7.055	1.00 18.34
ATOM	1491	CD2	TYR	A	251	25.076	39.018	8.852	1.00 16.39
ATOM	1492	CE1	TYR	A	251	26.819	40.984	7.955	1.00 18.20
ATOM	1493	CE2	TVD	Δ	251	25.622	39.925	9.753	
									1.00 17.81
MOTA	1494	CZ			251	26.487	40.900	9.302	1.00 17.43
MOTA	1495	OH	TYR	Α	251	27.014	41.779	10.215	1.00 20.25
ATOM	1496	N	THR	Δ	252	24.395	34.803	6.436	1.00 15.07
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ATOM	1497	CA			252	23.525	33.725	5.933	1.00 14.48
MOTA	1498	С	THR	Α	252	22.204	33.996	6.646	1.00 16.15
MOTA	1499	0	THR	A	252	22.193	34.429	7.845	1.00 16.66
ATOM	1500	СВ			252	24.056	32.325		
								6.330	1.00 14.69
ATOM	1501	OG1	THR	Ą	252	23.273	31.316	5.684	1.00 13.97
MOTA	1502	CG2	THR	Α	252	23.974	32.118	7.839	1.00 14.05
ATOM	1503	N	PRO	Δ	253	21.070	33.774	5.972	1.00 15.93
ATOM	1504	CA			253	19.826	34.054	6.694	1.00 17.09
MOTA	1505	C	PRO	Α	253	19.418	33.029	7.741	1.00 18.67
ATOM	1506	0	PRO	Α	253	19.782	31.813	7.653	1.00 17.11
ATOM	1507	СВ			253				
						18.789	34.161	5.572	1.00 17.20
ATOM	1508	CG	PRO	Α	253	19.304	33.207	4.545	1.00 17.18
ATOM	1509	CD	PRO	Α	253	20.809	33.468	4.553	1.00 17.14
ATOM	1510	N			254	18.692	33.501	8.750	1.00 18.82
MOTA	1511	CA			254	18.165	32.604	9.792	1.00 20.14
ATOM	1512	C	ILE	Α	254	16.885	32.091	9.137	1.00 21.33
ATOM	1513	0	TLE	Δ	254	15.911	32.875	8.914	1.00 21.52
ATOM	1514	CB	ILE			17.827	33.368	11.091	1.00 20.62
MOTA	1515	CG1	ILE	Α	254	19.124	33.752	11.806	1.00 20.82
MOTA	1516	CG2	ILE	Α	254	16.935	32.509	11.994	1.00 19.41
ATOM	1517	CD1				18.920	34.458		
								13.127	1.00 22.19
MOTA	1518	N	ARG	Α	255	16.868	30.810	8.795	1.00 22.06
ATOM	1519	CA	ARG	Α	255	15.702	30.211	8.115	1.00 23.47
ATOM	1520	С	ARG	Δ	255	14.398	30.343	8.880	1.00 24.68
ATOM	1521	0	ARG			13.334	30.719	8.299	1.00 25.49
MOTA	1522	CB	ARG	Α	255	15.951	28.735	7.852	1.00 22.62
MOTA	1523	CG	ARG	А	255	14.843	28.093	7.053	1.00 22.10
MOTA	1524	CD	ARG			14.985	26.598		
								7.069	1.00 22.76
ATOM	1525	NE	ARG	Α	255	14.031	25.958	6.176	1.00 22.51
MOTA	1526	CZ	ARG	A	255	13.692	24.679	6.256	1.00 22.37
MOTA	1527	NH1	ARG	Δ	255	14.232	23.914	7.195	1.00 20.91
	1528								
ATOM		NH2	ARG			12.819	24.166	5.396	1.00 23.78
ATOM	1529	N	ARG	A	256	14.451	30.023	10.165	1.00 24.98
MOTA	1530	CA	ARG	Α	256	13.264	30.085	11.029	1.00 25.56
ATOM	1531	С	ARG			13.723	30.441	12.438	1.00 24.84
ATOM	1532	0	ARG			14.829	30.013	12.893	1.00 22.14
MOTA	1533	CB	ARG	Α	256	12.561	28.729	11.009	1.00 27.37
ATOM	1534	CG	ARG			11.350	28.599	11.914	1.00 29.24
MOTA	1535	CD	ARG			10.878	27.150	11.899	1.00 29.60
ATOM	1536	NE	ARG	Α	256	10.180	26.788	13.126	1.00 31.29
ATOM	1537	CZ	ARG	Α	256	10.043	25.543	13.563	1.00 31.25
ATOM	1538		ARG						
						10.559	24.535	12.870	1.00 31.19
MOTA	1539	NHZ	ARG			9.398	25.307	14.698	1.00 32.97
MOTA	1540	N	GLU	A	257	12.914	31.219	13.141	1.00 24.01
MOTA	1541	CA	GLU			13.270	31.650	14.500	1.00 23.46
MOTA	1542	C	GLU			12.829	30.739	15.636	1.00 23.02
ATOM	1543	0	GLU	A	257	11.749	30.947	16.264	1.00 26.15
ATOM	1544	СВ	GLU	Α	257	12.739	33.055	14.748	1.00 23.25
ATOM	1545	CG							
			GLU			13.439	34.123	13.930	1.00 26.24
MOTA	1546	CD	GLU	Α	257	12.572	35.353	13.746	1.00 27.27

MOTA	1547	OE1	GLU A	257	13.124	36.470	13.673	1.00 27.35
ATOM	1548	OE2	GLU A		11.334	35.197	13.665	1.00 30.46
MOTA	1549 _.	N	TRP A		13.632	29.719	15.898	1.00 19.64
MOTA	1550	CA	TRP A	258	13.390	28.798	17.016	1.00 19.75
ATOM	1551	С	TRP A	258	14.812	28.548	17.495	1.00 19.46
			TRP A			29.190		
MOTA	1552	0			15.267		18.500	1.00 20.47
ATOM	1553	CB	TRP A	258	12.632	27.537	16.561	1.00 18.27
ATOM	1554	CG	TRP A	258	13.203	26.710	15.455	1.00 17.96
						27.143	14.364	
MOTA	1555	CD1	TRP A		13.898			1.00 18.43
MOTA	1556	CD2	TRP A	258	13.051	25.293	15.298	1.00 17.87
ATOM	1557	NE1	TRP A	258	14.187	26.082	13.537	1.00 18.62
ATOM	1558	CE2	TRP A		13.678	24.935	14.088	1.00 17.86
MOTA	1559.	CE3	TRP A		12.441	24.291	16.067	1.00 17.50
MOTA	1560	CZ2	TRP A	258	13.717	23.614	13.624	1.00 19.19
ATOM	1561	CZ3	TRP A	258	12.477	22.976	15.608	1.00 19.16
	1562	CH2	TRP A		13.113	22.650	14.396	1.00 18.86
MOTA								
MOTA	1563	N	TYR A		15.538	27.670	16.814	1.00 18.33
ATOM	1564	CA	TYR A	259	16.965	27.458	17.126	1.00 15.42
ATOM	1565	С	TYR A	259	17.550	28.474	16.157	1.00 16.46
	1566	Õ	TYR A		16.789	29.066	15.323	1.00 15.71
MOTA								
MOTA	1567	CB	TYR A	259	17.439	26.078	16.671	1.00 13.86
MOTA	1568	CG	TYR A	259 .	17.056	24.927	17.564	1.00 13.98
ATOM	1569	CD1	TYR A		17.876	24.539	18.627	1.00 13.32
			TYR A		15.875	24.224	17.346	1.00 12.14
MOTA	1570	CD2						
ATOM	1571	CE1	TYR A	259	17.520	23.467	19.450	1.00 15.06
ATOM	1572	CE2	TYR A	259	15.510	23.167	18.155	1.00 14.24
ATOM	1573	CZ	TYR A		16.329	22.789	19.200	1.00 14.26
MOTA	1574	OH	TYR A		15.940	21.719	19.955	1.00 12.92
MOTA	1575	N	TYR A	260	18.851	28.725	16.224	1.00 14.50
ATOM	1576	CA	TYR A	260	19.440	29.630	15.232	1.00 15.21
ATOM	1577	С	TYR A		19.716	28.718	14.037	1.00 15.90
MOTA	1578	0	TYR A		20.866	28.210	13.836	1.00 16.76
ATOM	1579	CB	TYR A	260	20.722	30.269	15.759	1.00 13.84
ATOM	1580	CG	TYR A	260	20.426	31.416	16.690	1.00 14.32
ATOM	1581	CD1	TYR A		20.534	31.270	18.078	1.00 13.41
MOTA	1582	CD2	TYR A		19.996	32.642	16.187	1.00 13.45
MOTA	1583	CE1	TYR A	260	20.224	32.320	18.933	1.00 13.15
ATOM	1584	CE2	TYR A	260	19.680	33.699	17.037	1.00 12.56
ATOM	1585	CZ	TYR A		19.801	33.530	18.404	1.00 13.22
							19.239	1.00 12.88
MOTA	1586	ОН	TYR A		19.531	34.582		
MOTA	1587	N	GLU A	261	18.664	28.476	13.260	1.00 15.81
MOTA	1588	CA	GLU A	261	18.741	27.586	12.081	1.00 17.54
ATOM	1589	С	GLU A		19.191	28.266	10.791	1.00 17.31
	_					29.355		1.00 16.63
MOTA	1590	0	GLU A		18.665		10.402	
MOTA	1591	CB	GLU A	261	17.382	26.914	11.842	1.00 16.53
MOTA	1592	CG	GLU A	261	17.326	26.076	10.573	1.00 19.47
ATOM	1593	CD	GLU A		15.965	25.454	10.326	1.00 20.18
								1.00 21.27
MOTA	1594	OE1			14.956	26.037	10.766	
MOTA	1595	OE2	GLU A	261	15.902	24.390	9.673	1.00 20.94
ATOM	1596	N	VAL A	262	20.153	27.640	10.122	1.00 16.45
ATOM	1597	CA	VAL A		20.679	28.147	8.842	1.00 16.13
ATOM	1598	C	VAL A		20.620	27.006	7.831	1.00 17.33
ATOM	1599	σ	VAL A	262	20.168	25.863	8.166	1.00 17.30
MOTA	1600	СВ	VAL A	262	22.131	28.624	8.982	1.00 14.58
			VAL A		22.218	29.690	10.064	1.00 14.84
ATOM	1601							
MOTA	1602	CG2	VAL A		23.039	27.449	9.308	1.00 14.53
ATOM	1603	N	ILE A	263	21.064	27.271	6.608	1.00 17.34
ATOM	1604	CA	ILE A	263	21.044	26.245	5.554	1.00 16.67
ATOM	1605		ILE A		22.419	26.042	4.931	1.00 16.64
		С						1.00 17.50
MOTA	1606	0	ILE A		23.054	27.016	4.418	
MOTA	1607	CB	ILE A	263	20.031	26.619	4.445	1.00 18.45
MOTA	1608	CG1	ILE A	263	18.608	26.522	4.996	1.00 18.90

ATOM	1609	CG2	ILE A		20.192	25.694	3.243	1.00 18.17
ATOM	1610	CD1	ILE A	263	17.541	26.974	4.023	1.00 23.31
ATOM	1611	N	ILE A		22.897	24.802	4.988	1.00 16.67
	-							
MOTA	1612	CA	ILE A		24.199	24.413	4.409	1.00 14.63
ATOM	1613	С	ILE A	264	23.882	23.836	3.031	1.00 16.44
MOTA	1614	0	ILE A	264	23.019	22.915	2.908	1.00 13.53
					-			
ATOM.	1615	CB	ILE A		24.877	23.320	5.253	1.00 14.79
ATOM	1616	CG1	ILE A	264	25.174	23.855	6.657	1.00 12.53
ATOM	1617	CG2	ILE A	264	26.154	22.846	4.563	1.00 12.07
ATOM	1618′	CD1	ILE A		25.685	22.799	7.615	1.00 12.69
ATOM	1619	N	VAL A	265	24.546	24.334	1.992	1.00 17.37
ATOM	1620	CA	VAL A	265	24.258	23.841	0.627	1.00 18.64
ATOM	1621	C	VAL A		25.368	23.004	0.006	1.00 19.95
ATOM	1622	0	VAL A	265	25.202	22.455	-1.127	1.00 19.29
ATOM	1623	CB	VAL A	265	23.956	25.011	-0.322	1.00 18.56
ATOM	1624	CG1	VAL A	265	22.874	25.901	0.287	1.00 16.70
	1625	CG2	VAL A		25.227	25.802	-0.590	1.00 17.47
MOTA								
MOTA	1626	N	ARG A	266	26.486	22.872	0.707	1.00 20.42
ATOM	1627	CA	ARG A	266	27.617	22.098	0.165	1.00 20.48
ATOM	1628	С	ARG A		28.752	22.044	1.162	1.00 19.59
MOTA	1629	0	ARG A		29.030	23.055	1.885	1.00 19.51
ATOM	1630	CB	ARG A	266	28.112	22.763	-1.129	1.00 22.33
ATOM	1631	CG	ARG A	266	29.417	22.218	-1.713	1.00 22.40
ATOM	1632	CD	ARG A		29.939	23.170	-2.789	1.00 24.49
ATOM	1633	NE	ARG A		31.244	22.785	-3.322	1.00 24.49
ATOM	1634	CZ	ARG A	266	31.444	22.266	-4.528	1.00 26.46
ATOM	1635	NH1	ARG A	266	30.426	22.061	-5.349	1.00 25.31
ATOM	1636	NH2	ARG A		32.672	21.956	-4.920	1.00 27.88
ATOM	1637	N	VAL A	267	29.404	20.891	1.246	1.00 18.31
ATOM	1638	CA	VAL A	267	30.561	20.766	2.136	1.00 18.32
ATOM	1639	С	VAL A	267	31.671	20.072	1.369	1.00 18.25
								1.00 19.14
MOTA	1640	0	VAL A		31.409	19.192	0.489	
MOTA	1641	CB	VAL A	267	30.248	19.974	3.456	1.00 18.72
ATOM	1642	CG1	VAL A	267	28.784	19.645	3.547	1.00 18.30
ATOM	1643		VAL A		31.112	18.728	3.554	1.00 17.65
MOTA	1644	N	GLU A		32.903	20.471	1.647	1.00 16.18
MOTA	1645	CA	GLU A	268	34.046	19.848	0.990	1.00 17.71
ATOM	1646	С	GLU A	268	35.169	19.546	1.970	1.00 16.08
ATOM	1647	ō	GLU A		35.293	20.191	3.064	1.00 13.62
MOTA	1648	CB	GLU A		34.550	20.717	-0.177	1.00 18.50
ATOM	1649	CG	GLU A	268	34.430	22.207	0.030	1.00 22.46
ATOM	1650	CD	GLU A	268	34.888	23.016	-1.181	1.00 22.13
ATOM	1651	OE1	GLU A		34.216	22.970	-2.237	1.00 20.91
ATOM	1652	OE2	GLU A		35.927	23.703	-1.067	1.00 22.44
MOTA	1653	N	ILE A	269	35.948	18.531	1.623	1.00 13.57
ATOM	1654	CA	ILE A	269	37.103	18.112	2.418	1.00 13.89
MOTA	1655	C			38.259	18.448	1.485	1.00 14.06
			ILE A					
MOTA	1656	0	ILE A	269	38.396	17.832	0.386	1.00 14.03
MOTA	1657	CB	ILE A	269	37.051	16.596	2.703	1.00 14.48
ATOM	1658	CG1			35.697	16.239	3.327	1.00 14.59
ATOM	1659		ILE A		38.180	16.193	3.645	1.00 12.12
ATOM	1660	CD1	ILE A	269	35.358	17.022	4.592	1.00 13.16
ATOM	1661	N	ASN A	270	39.067	19.431	1.872	1.00 14.16
ATOM	1662	CA	ASN A		40.205	19.886	1.038	1.00 13.20
								1.00 13.24
MOTA	1663	C	ASN A		39.774	20.177	-0.399	
MOTA	1664	0	ASN A	270	40.427	19.714	-1.385	1.00 13.72
MOTA	1665	СВ	ASN A	270	41.336	18.852	1.047	1.00 11.19
ATOM	1666	CG	ASN A		42.424	19.186	2.054	1.00 13.23
								1.00 13.62
MOTA	1667		ASN A		42.339	20.224	2.790	
ATOM	1668	ND2	ASN A	270	43.454	18.348	2.117	1.00 11.67
ATOM	1669	N	GLY A	271	38.691	20.932	-0.540	1.00 13.07
MOTA	1670	CA	GLY A		38.210	21.302	-1.858	1.00 13.58
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ATOM	1671	С	GLY	Α	271	37.393	20.241	-2.564	1.00 14.87
MOTA	1672	0			271	36.704	20.545	-3.581	1.00 13.70
ATOM	1673.				272	37.447	19.005	-2.076	1.00 14.64
MOTA	1674	CA			272	36.674	17.914	-2.705	1.00 14.45
ATOM	1675	C			272	35.261	17.870	-2.140	1.00 15.83
ATOM ATOM	1676 1677	O CB			272 272	35.050	17.717	-0.902	1.00 15.81
ATOM	1678	CG			272	37.357 36.692	16.561 15.421	-2.486 -3.250	1.00 14.85
ATOM	1679	CD			272	37.499	14.135	-3.211	1.00 14.45 1.00 16.34
ATOM	1680	0E1			272	37.097	13.134	-2.535	1.00 10.34
ATOM	1681	NE2			272	38.633	14.121	-3.909	1.00 13.09
ATOM	1682	N	ASP	A	273	34.291	17.995	-3.035	1.00 16.17
MOTA	1683	CA			273	32.857	17.987	-2.686	1.00 17.89
MOTA	1684	С			273	32.388	16.612	-2.201	1.00 16.92
ATOM	1685	0	ASP			32.713	15.566	-2.831	1.00 16.53
ATOM	1686	CB	ASP			32.060	18.395	-3.930	1.00 20.38
ATOM ATOM	1687 1688	CG OD1	ASP ASP			30.576	18.526	-3.665	1.00 20.89
ATOM	1689	OD1	ASP			29.827 30.155	18.788 18.378	-4.630 -2.503	1.00 21.98
ATOM	1690	N	LEU			31.639	16.576	-2.303 -1.101	1.00 22.40 1.00 17.95
ATOM	1691	CA	LEU			31.117	15.285	-0.587	1.00 17.33
ATOM	1692	С	LEU	Α	274	30.092	14.805	-1.598	1.00 21.18
MOTA	1693	0	LEU	Α	274	29.702	13.603	-1.623	1.00 20.08
MOTA	1694	CB	LEU			30.451	15.455	0.783	1.00 18.46
ATOM	1695	CG	LEU			31.356	15.595	2.011	1.00 19.89
ATOM	1696		LEU			30.489	15.558	3.267	1.00 17.23
ATOM ATOM	1697 1698		LEU LYS			32.392	14.463	2.050	1.00 17.76
ATOM	1699	N CA	LYS			29.646 28.676	15.736 15.452	-2.431 -3.501	1.00 24.29 1.00 29.08
ATOM	1700	C	LYS			27.439	14.715	-3.000	1.00 29.08
ATOM	1701	ō	LYS			27.119	13.586	-3.464	1.00 30.50
ATOM	1702	СВ	LYS			29.360	14.642	-4.608	1.00 30.50
ATOM	1703	CG	LYS	A	275	28.720	14.818	-5.970	1.00 33.82
ATOM	1704	CD	LYS	A	275	29.476	14.059	-7.042	1.00 36.63
ATOM	1705	CE.	LYS			28.848	14.297	-8.408	1.00 38.29
ATOM	1706	NZ	LYS			28.742	15.759	-8.702	1.00 39.43
MOTA MOTA	1707 1708	N	MET			26.734	15.329	-2.063	1.00 30.55
ATOM	1708	CA	MET MET		_	25.519 24.319	14.722 15.592	-1.505	1.00 30.03
ATOM	1710	0	MET			24.465	16.818	-1.815 -2.117	1.00 30.11 1.00 28.94
ATOM	1711	СВ	MET			25.641	14.576	0.011	1.00 20.34
ATOM	1712	CG	MET			26.706	13.605	0.469	1.00 30.69
MOTA	1713	SD	MET	A	276	26.687	13.418	2.261	1.00 32.94
MOTA	1714	CE	MET	A	276	25.174	12.457	2.477	1.00 31.04
MOTA	1715	N	ASP			23.136	14.994	-1.756	1.00 31.37
ATOM	1716	CA	ASP .			21.906	15.750	-1.994	1.00 33.34
ATOM ATOM	1717	C	ASP			21.903	16.864	-0.955	1.00 33.96
ATOM	1718 1719	O CB	ASP .			22.070 20.682	16.608	0.278 -1.818	1.00 30.80 1.00 36.24
ATOM	1720	CG	ASP .			19.377	14.851 15.595	-2.029	1.00 38.24
ATOM	1721		ASP .			18.332	14.925	-2.168	1.00 38.93
ATOM	1722		ASP .			19.386	16.844	-2.049	1.00 39.38
ATOM	1723	N	CYS .			21.732	18.089	-1.432	1.00 34.50
ATOM	1724	CA	CYS .	A	278	21.725	19.294	-0.581	1.00 37.44
MOTA	1725	С	CYS .			20.988	19.126	0.749	1.00 35.96
ATOM	1726	0	CYS			21.503	19.540	1.834	1.00 34.38
ATOM	1727	CB	CYS .			21.108	20.460	-1.362	1.00 39.86
ATOM ATOM	1728	SG	CYS			21.760	22.075	-0.852	1.00 50.09
ATOM ATOM	1729 1730	N CA	LYS :			19.802	18.529	0.705	1.00 33.76 1.00 32.65
ATOM	1731	CA	LYS A			19.003 19.584	18.359 17.430	1.931 2.996	1.00 32.65
ATOM	1732	Ö	LYS 2			19.173	17.501	4.189	1.00 27.89
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MOTA	1733	CB	LYS A	279	17.574	17.939	1.567	1.00 34.74
MOTA	1734	CG	LYS A		17.459	16.765	0.612	1.00 39.08
MOTA	1735	CD	LYS A		17.576	15.429	1.326	1.00 41.32
ATOM	1736	CE	LYS A	. 279	17.185	14.289	0.393	1.00 42.86
ATOM	1737	NZ	LYS A	279	17.118	12.978	1.099	1.00 45.07
MOTA	1738	N	GLU A		20.525	16.570	2.621	1.00 27.06
ATOM	1739	CA	GLU A	280	21.141	15.659	3.612	1.00 26.22
ATOM	1740	С	GLU A	280	21.900	16.458	4.673	1.00 25.34
							5.886	
ATOM	1741	0	GLU A		21.920	16.074		1.00 23.01
ATOM	1742	CB	GLU A	. 280	22.109	14.693	2.928	1.00 27.98
MOTA	1743	CG	GLU A	280	21.459	13.725	1.946	1.00 31.24
ATOM	1744	CD	GLU A		20.486	12.765	2.610	1.00 32.55
ATOM	1745	OE1	GLU A		20.447	12.704	3.857	1.00 33.21
MOTA	1746	OE2	GLU A	. 280	19.763	12.058	1.878	1.00 34.72
ATOM	1747	N	TYR A	281	22.515	17.562	4.255	1.00 23.32
		CA	TYR A		23.295	18.420	5.176	1.00 22.69
MOTA	1748							
ATOM	1749	С	TYR A		22.415	19.082	6.219	1.00 23.40
ATOM	1750	0	TYR A	281	22.904	19.470	7.327	1.00 23.11
MOTA	1751	CB	TYR A		24.035	19.515	4.400	1.00 20.26
					24.958	18.993	3.328	1.00 19.39
MOTA	1752	CG	TYR A					
ATOM	1753	CD1	TYR A	. 281	25.858	17.961	3.601	1.00 17.78
MOTA	1754	CD2	TYR A	281	24.943	19.534	2.042	1.00 18.55
MOTA	17:55	CE1	TYR A	281	26.719	17.478	2.623	1.00 17.05
								1.00 18.53
MOTA	1756	CE2	TYR A		25.808	19.058	1.051	
ATOM	1757	ÇΖ	TYR A	. 281	26.692	18.028	1.355	1.00 17.87
ATOM	1758	OH	TYR A	281	27.558	17.533	0.407	1.00 18.13
MOTA		. N	ASN A		21.136	19.232	5.899	1.00 22.82
							6.820	1.00 23.17
ATOM	1760	CA	ASN A		20.194	19.881		
MOTA	1761	С	ASN A	282	19.089	18.922	7.238	1.00 23.84
ATOM	1762	0	ASN A	282	17.987	19.366	7.685	1.00 21.83
MOTA	1763	CB	ASN A		19.598	21.111	6.137	1.00 22.42
								1.00 23.90
MOTA	1764	CG	ASN A		20.665	22.018	5.549	
MOTA	1765	OD1	ASN A	282	21.426	22.693	6.298	1.00 23.87
MOTA	1766	ND2	ASN A	282	20.760	22.044	4.224	1.00 23.36
ATOM	1767	N	TYR A		19.343	17.623	7.102	1.00 25.74
							7.472	1.00 28.01
ATOM	1768	CA	TYR A	_	18.322	16.633		
MOTA	1769	С	TYR A	283	17.905	16.843	8.912	1.00 29.29
ATOM	1770	0	TYR A	283	18.686	16.572	9.881	1.00 27.50
MOTA	1771	CB	TYR A	283	18.810	15.200	7.280	1.00 29.52
		CG	TYR A		17.783	14.200	7.756	1.00 31.64
MOTA	1772							
ATOM	1773	CD1			16.428	14.374	7.460	1.00 32.38
ATOM	1774	CD2	TYR A	283	18.153	13.098	8.523	1.00 33.44
ATOM	1775	CE1	TYR A	283	15.468	13.479	7.919	1.00 33.96
	•				17.201	12.194	8.987	1.00 35.48
ATOM	1776		TYR A					
MOTA	1777	CZ	TYR A	283	15.860	12.392	8.683	1.00 35.35
ATOM	1778	OH	TYR A	283	14.918	11.504	9.149	1.00 36.54
ATOM	1779	N	ASP A		16.665	17.299	9.043	1.00 30.23
			ASP A		16.026	17.638	10.312	1.00 28.41
ATOM	1780	CA						
MOTA	1781	С	ASP A		16.273	19.129	10.409	1.00 27.12
ATOM	1782	0	ASP A	284	15.309	19.953	10.305	1.00 25.19
MOTA	1783	CB	ASP A		16.684	16.928	11.494	1.00 33.07
							12.813	1.00 33.49
MOTA	1784	CG	ASP A		16.035	17.283		
MOTA	1785	DD1	ASP A	284	16.520	16.815	13.860	1.00 37.38
MOTA	1786	OD2	ASP A	284	15.035	18.031	12.802	1.00 35.95
ATOM	1787	N	LYS A		17.542	19.499	10.563	1.00 22.62
								1.00 20.42
MOTA	1788	CA	LYS A		17.914	20.927	10.678	
MOTA	1789	С	LYS A		19.420	21.145	10.812	1.00 19.89
MOTA	1790	0	LYS A		20.209	20.174	11.037	1.00 19.63
ATOM	1791	CB	LYS A		17.230	21.540	11.903	1.00 18.63
							13.232	1.00 16.63
ATOM	1792	CG	LYS A		17.753	20.987		
ATOM	1793	CD	LYS A		16.966	21.538	14.421	1.00 14.93
MOTA	1794	CE	LYS 2	285	17.551	21.088	15.754	1.00 15.57

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MOTA	1795	ΝZ	LYS	Α	285	17.482	19.606	15.974	1.00 13.50
ATOM	1796	N	SER	Α	286	19.827	22.402	10.678	1.00 17.19
MOTA	1797	CA			286	21.241	22.808	10.827	
									1.00 16.52
MOTA	1798	С	SER	Α	286	21.228	24.034	11.727	1.00 15.74
ATOM	1799	0	SER	Α	286	20.592	25.080	11.377	1.00 14.46
ATOM	1800	CB	SER	Α	286	21.862	23.179	9.475	1.00 16.90
					286				
ATOM	1801	OG				22.064	22.036	8.671	1.00 16.60
ATOM	1802	N	ILE	A	287	21.900	23.946	12.870	1.00 13.25
ATOM	1803	CA	ILE	Α	287	21.933	25.079	13.805	1.00 13.97
ATOM	1804	С	TLE	А	287	23.342	25.511	14.206	1.00 15.14
ATOM	1805	ō			287	24.346	24.750	14.024	1.00 14.63
MOTA	1806	CB			287	21.145	24.757	15.102	1.00 13.55
MOTA	1807	CG1	ILE	Α	287	21.898	23.717	15.929	1.00 12.52
ATOM	1808	CG2	ILE	Α	287	19.758	24.214	14.754	1.00 12.10
ATOM	1809	CD1	ILE	Α	287	21.274	23.455	17.283	1.00 14.43
ATOM	1810	N			288	23.431	26.728	14.732	1.00 14.78
						24.701	27.292		
ATOM	1811	CA			288			15.223	1.00 15.54
MOTA	1812	С			288	24.510	27.262	16.733	1.00 16.05
MOTA	1813	Ο.	VAL	Α	288	23.571	27.930	17.278	1.00 15.61
ATOM	1814	CB	VAL	Α	288	24.896	28.751	14.767	1.00 15.19
ATOM	1815	CG1	VAL	Α	288	26.248	29.259	15.239	1.00 14.78
ATOM	1816		VAL			24.791	28.842	13.246	1.00 15.19
MOTA	1817	N			289	25.355	26.512	17.430	1.00 15.91
MOTA	1818	CA	ASP	A	289	25.194	26.373	18.891	1.00 14.81
ATOM	1819	С	ASP	Α	289	26.467	26.444	19.724	1.00 15.27
ATOM	1820	0	ASP	Α	289	27.322	25.504	19.700	1.00 15.75
ATOM	1821	ĊВ			289	24.467	25.060	19.168	1.00 12.65
ATOM	1822	CG			289	24.264	24.806	20.634	1.00 13.29
MOTA	1823	OD1	ASP			24.372	25.768	21.426	1.00 11.88
ATOM	1824	OD2	ASP	Α	289	23.981	23.639	20.988	1.00 10.63
MOTA	1825	N	SER	А	290	26.604	27.529	20.479	1.00 15.19
ATOM	1826	CA			290	27.782	27.730	21.346	1.00 14.55
ATOM	1827	С			290	27.770	26.748	22.510	1.00 15.43
MOTA	1828	0	SER	Α	290	28.823	26.539	23.186	1.00 13.77
ATOM	1829	CB	SER	Α	290	27.795	29.165	21.888	1.00 15.33
ATOM	1830	OG	SER	Α	290	26.614	29.442	22.620	1.00 12.79
ATOM	1831	N			291	26.612	26.137	22.759	1.00 14.34
ATOM	1832	CA			291	26.486	25.192	23.856	1.00 14.93
ATOM	1833	С	GLY			26.779	23.751	23.479	1.00 16.64
ATOM	1834	0	GLY	Α	291	26.502	22.792	24.277	1.00 14.49
ATOM	1835	N	THR	A	292	27.305	23.556	22.277	1.00 16.47
ATOM	1836	CA	THR			27.674	22.202	21.812	1.00 15.30
ATOM	1837	C	THR			29.159	22.215	21.482	1.00 14.67
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ATOM	1838	0			292	29.653	23.102	20.725	1.00 13.26
ATOM	1839	CB	THR	A	292	26.889	21.784	20.550	1.00 15.29
ATOM	1840	OG1	THR	Α	292	25.522	21.521	20.895	1.00 13.88
ATOM	1841	CG2	THR	Α	292	27.514	20.527	19.932	1.00 13.59
ATOM	1842	N	THR			29.887	21.253	22.027	1.00 14.43
			THR					21.801	1.00 12.76
ATOM	1843	CA				31.343	21.162		
ATOM	1844	С	THR			31.749	20.906	20.348	1.00 14.47
ATOM	1845	0	THR	Α	293	32.478	21.735	19.712	1.00 14.61
MOTA	1846	CB	THR	Α	293	31.949	20.035	22.650	1.00 12.36
ATOM	1847		THR			31.726	20.304	24.041	1.00 10.79
	1848		THR			33.437	19.916	22.382	1.00 9.56
ATOM									
MOTA	1849	N	ASN			31.286	19.783	19.810	1.00 13.53
MOTA	1850	CA	ASN			31.648	19.349	18.440	1.00 15.26
MOTA	1851	C	ASN	Α	294	30.871	19.917	17.276	1.00 15.45
MOTA	1852	0	ASN			29.851	20.662	17.431	1.00 13.68
ATOM	1853	СВ			294	31.494	17.832	18.307	1.00 14.81
	1854	CG			294	32.351	17.051	19.270	1.00 14.13
ATOM								19.304	1.00 19.85
MOTA	1855		ASN			32.264	15.791		
ATOM	1856	NDZ	ASN	A	294	33.174	17.734	20.051	1.00 13.25

ATOM	1857	N	LEU	Α	295	31.365	19.556	16.096	1.00 15.21
ATOM	1858	CA			295	30.689	19.866		
								14.835	1.00 15.29
ATOM	1859.	С	LEU	Α	295	29.924	18.548	14.719	1.00 16.43
ATOM	1860	0	T. ETT	Δ	295	30.556	17.452	14.575	1.00 16.34
ATOM	1861	CB	LEU	Α	295	31.674	19.963	13.671	1.00 13.54
ATOM	1862	CG	T.PIT	Δ	295	31.017	19.837	12.287	1.00 14.74
MOTA	1863	CDI	LEU	Α	295	29.991	20.947	12.109	1.00 14.37
ATOM	1864	CD2	LEU	Δ	295	32.073	19.903	11.179	1.00 13.91
ATOM	1865	N	ARG	A.	296	28.606	18.591	14.831	1.00 16.08
ATOM	1866	CA	ARG	Δ	296	27.827	17.349	14.719	1.00 17.47
ATOM	1867	С	ARG	A	296	27.180	17.300	13.343	1.00 17.04
ATOM	1868	0	ARG	Α	296	26.655	18.339	12.840	1.00 15.28
	1869				296	26.785			
ATOM'	-	СВ					17.290	15.834	1.00 18.37
MOTA	1870	CG	ARG	Α	296	27.421	17.444	17.208	1.00 19.73
ATOM	1871	CD	ARC	Δ	296	26.425	17.262	18.324	1.00 22.63
MOTA	1872	NE	ARG	A	296	26.292	15.867	18.722	1.00 25.23
MOTA	1873	cz	ARG	Α	296	25.135	15.223	18.776	1.00 26.52
MOTA	1874		ARG			24.011	15.851	18.446	1.00 27.11
ATOM	1875	NH2	ARG	Α	296	25.100	13.961	19.179	1.00 27.00
ATOM	1876	N	T.DIT	70	297	27.211	16.123	12.722	1.00 15.65
ATOM	1877	CA	LEU	Α	297	26.660	15.945	11.356	1.00 15.33
MOTA	1878	С	LEU	Α	297	25.657	14.800	11.246	1.00 17.46
MOTA	1879	0	LEU	A	297	25.795	13.743	11.938	1.00 16.37
ATOM	1880	CB	LEU	Α	297	27.806	15.681	10.371	1.00 12.00
MOTA	1881	CG	LEU			28.925	16.729	10.277	1.00 11.84
ATOM	1882	CD1	LEU	Α	297	30.136	16.148	9.561	1.00 8.16
MOTA	1883	CD2	LEU	Δ	297	28.410	17.962	9.559	1.00 8.99
ATOM	1884	N	PRO	Α	298	24.636	14.960	10.386	1.00 19.11
ATOM	1885	CA	PRO	Α	298	23.636	13.901	10.217	1.00 20.53
MOTA	1886	С	PRO			24.387	12.619	9.868	1.00 21.03
ATOM	1887	0	PRO	Α	298	25.419	12.668	9.131	1.00 21.77
ATOM	1888	CB	PRO	7	200	22.788	14.411	9.054	1.00 19.18
ATOM	1889	ÇG	PRO	Α	298	22.861	15.897	9.209	1.00 20.46
MOTA	1890	CD	PRO	Δ	298	24.335	16.111	9.517	1.00 19.69
ATOM	1891	N	LYS	A	299	23.911	11.487	10.376	1.00 22.77
MOTA	1892	CA	LYS	Α	299	24.562	10.169	10.137	1.00 25.34
	1893	C	LYS				9.979	8.753	1.00 24.56
ATOM						25.169			
ATOM	1894	0	LYS	Α	299	26.393·	9.681	8.617	1.00 22.24
ATOM	1895	CB	LYS	Δ	299	23.566	9.034	10.387	1.00 29.05
ATOM	1896	CG	LYS			24.156	7.650	10.146	1.00 33.27
ATOM	1897	CD	LYS	Α	299	23.144	6.547	10.408	1.00 37.10
MOTA	1898	CE	LYS			23.758	5.178	10.151	1.00 38.78
MOTA	1899	NZ	LYS	Α	299	22.775	4.077	10.380	1.00 42.51
ATOM	1900	N	LYS	Α	300	24.340	10.127	7.729	1.00 24.24
MOTA	1901	CA	LYS			24.774	9.955	6.333	1.00 25.41
ATOM	1902	С	LYS	Α	300	25.901	10.916	5.952	1.00 24.12
MOTA	1903	0	LYS	Δ	300	26.889	10.515	5.262	1.00 23.67
MOTA	1904	СB	LYS	A	300	23.576	10.154	5.403	1.00 28.77
ATOM	1905	CG	LYS	Α	300	23.788	9.660	3.990	1.00 33.37
MOTA	1906	CD	LYS	A	300	22.661	8.718	3.569	1.00 38.01
MOTA	1907	CE	LYS	Α	300	21.298	9.393	3.652	1.00 40.18
ATOM	1908	NZ	LYS			20.191	8.455	3.291	1.00 42.69
MOTA	1909	N	VAL	Α	301	25.784	12.172	6.368	1.00 20.46
ATOM	1910	CA	VAL	Α	301	26.832	13.169	6.058	1.00 18.21
MOTA	1911	С	VAL			28.083	12.842	6.867	1.00 17.93
ATOM	1912	0	VAL	Α	301	29.241	12.929	6.343	1.00 16.84
ATOM	1913	СВ	VAL			26.358	14.601	6.391	1.00 17.29
ATOM	1914		VAL			27.468	15.605	6.105	1.00 15.43
ATOM	1915		VAL			25.118	14.935	5.565	1.00 16.34
MOTA	1916	N	PHE			27.887	12.448	8.122	1.00 17.43
ATOM	1917	CA	PHE	Α	302	29.032	12.099	8.990	1.00 18.16
ATOM	1918	C	PHE			29.854	10.957	8.399	1.00 18.95
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MOTA	1919	0	PHE A	302	31.121	11.004	8.399	1.00 18.60
MOTA	1920	CB	PHE A	302	28.550	11.713	10.391	1.00 17.38
						11.180	11.265	1.00 19.16
MOTA	1921 -		PHE A		29.639			
MOTA	1922	CD1	PHE A	302	29.866	9.810	11.362	1.00 17.81
	1923	CD2	PHE A	302	30.498	12.051	11.923	1.00 18.89
MOTA								
MOTA	1924	CEl	PHE A	302	30.934	9.320	12.096	1.00 19.63
MOTA	1925	CE2	PHE A	302	31.573	11.569	12.660	1.00 19.90
							12.747	1.00 19.13
MOTA	1926	CZ	PHE A		31.793	10.201		
MOTA	1927	N	GLU A	303	29.172	9.931	7.901	1.00 19.20
	1928	CA	GLU A		29.859	8.769	7.295	1.00 21.56
MOTA								
ATOM	1929	С	GLU A	303	30.679	9.189	6.083	1.00 19.19
MOTA	1930	0	GLU A	303	31.865	8.777	5.929	1.00 18.04
						7.704	6.888	1.00 24.72
MOTA	1931	CB	GLU A		28.836			
ATOM	1932	CG	GLU A	303	28.246	6.939	8.069	1.00 29.90
ATOM	1933	CD	GLU A		27.051	6.076	7.683	1.00 33.77
						5.294	8.541	1.00 36.31
MOTA	1934		GLU A		26.585			
MOTA	1935	OE2	GLU A	303	26.572	6.183	6.528	1.00 36.51
MOTA	1936	N	ALA A		30.088	9.998	5.216	1.00 17.86
MOTA	1937	CA	ALA A	304	30.805	10.472	4.007	1.00 18.11
ATOM	1938	С	ALA A	304	31.999	11.354	4.386	1.00 17.49
	1939	ō	ALA A		33.102	11.242	3.777	1.00 17.76
ATOM								
MOTA	1940	CB	ALA A	304	29.849	11.244	3.102	1.00 17.14
ATOM	1941	N	ALA A	305	31.812	12.221	5.377	1.00 17.06
					32.900	13.128	5.829	1.00 16.43
MOTA	1942	CA	ALA A					
ATOM	1943	С	ALA A	305	34.092	12.387	6.440	1.00 16.39
ATOM	1944	0	ALA A	305	35.272	12.644	6.054	1.00 17.78
						14.140	6.833	1.00 15.92
MOTA	1945	CB	ALA A		32.351			
ATOM	1946	N	VAL A	306	33.842	11.476	7.375	1.00 15.50
MOTA	1947	CA	VAL A	306	34.971	10.756	8.004	1.00 17.31
							6.987	1.00 16.95
MOTA	1948	С	VAL A	306	35.719	9.920		
MOTA	1949	0	VAL A	306	36.983	9.829	7.029	1.00 16.21
	1950	СВ	VAL A		34.514	9.845	9.162	1.00 17.93
MOTA								
MOTA	1951	CG1	VAL A	306	33.954	10.693	10.280	1.00 19.37
ATOM	1952	CG2	VAL A	306	33.477	8.851	8.669	1.00 19.63
			LYS A		34.987	9.307	6.065	1.00 17.11
MOTA	1953	N						
MOTA	1954	CA	LYS A	307	35.641	8.488	5.032	1.00 18.39
ATOM	1955	С	LYS A	307	36.654	9.350	4.279	1.00 17.59
					37.848	8.959	4.107	1.00 18.09
MOTA	1956	0	LYS A					
ATOM	1957	CB	LYS A	307	34.602	7.940	4.052	1.00 19.72
ATOM	1958	CG	LYS A	307	35.212	7.112	2.930	1.00 24.02
					34.147	6.415	2.102	1.00 26.72
MOTA	1959	CD	LYS A					
ATOM	1960	CE	LYS A	307	34 <i>.</i> 779	5.505	1.058	1.00 29.36
ATOM	1961	NZ	LYS A	307	33.745	4.869	0.193	1.00 31.68
					36.205	10.520	3.842	1.00 16.75
ATOM	1962	N	SER A					
ATOM	1963	CA	SER A	308	37.059	11.460	3.091	1.00 17.46
ATOM	1964	C	SER A		38.198	12.000	3.953	1.00 16.11
					39.378		3.501	1.00 17.12
MOTA	1965	0	SER A			12.056		
MOTA	1966	CB	SER A	308	36.208	12.620	2.560	1.00 17.51
MOTA	1967	OG	SER A		36.982	13.505	1.774	1.00 19.76
							5.180	1.00 16.07
MOTA	1968	N	ILE A		37.886	12.400		
MOTA	1969	CA	ILE A	309	38.926	12.927	6.083	1.00 14.41
ATOM			ILE A		39.945	11.831	6.378	1.00 14.93
	1970							
MOTA	1970	Ċ						
	1970 1971	.0	ILE A	309	41.171	12.112	6.505	1.00 14.90
ATOM	1971		ILE A	309				
ATOM	1971 1972	O CB	ILE A	309 309	41.171 38.310	12.112 13.439	6.505 7.401	1.00 14.90 1.00 13.88
MOTA	1971 1972 1973	O CB CG1	ILE A ILE A ILE A	309 309 309	41.171 38.310 37.346	12.112 13.439 14.595	6.505 7.401 7.099	1.00 14.90 1.00 13.88 1.00 13.08
	1971 1972	O CB CG1 CG2	ILE A ILE A ILE A	309 309 309 309	41.171 38.310 37.346 39.404	12.112 13.439 14.595 13.887	6.505 7.401 7.099 8.350	1.00 14.90 1.00 13.88 1.00 13.08 1.00 11.40
ATOM ATOM	1971 1972 1973 1974	O CB CG1 CG2	ILE A ILE A ILE A	309 309 309 309	41.171 38.310 37.346	12.112 13.439 14.595	6.505 7.401 7.099	1.00 14.90 1.00 13.88 1.00 13.08 1.00 11.40 1.00 12.70
ATOM ATOM ATOM	1971 1972 1973 1974 1975	O CB CG1 CG2 CD1	ILE A ILE A ILE A ILE A	309 309 309 309 309	41.171 38.310 37.346 39.404 36.575	12.112 13.439 14.595 13.887 15.084	6.505 7.401 7.099 8.350 8.315	1.00 14.90 1.00 13.88 1.00 13.08 1.00 11.40 1.00 12.70
MOTA MOTA MOTA MOTA	1971 1972 1973 1974 1975	O CB CG1 CG2 CD1 N	ILE A ILE A ILE A ILE A ILE A ILE A	309 309 309 309 309 310	41.171 38.310 37.346 39.404 36.575 39.475	12.112 13.439 14.595 13.887 15.084 10.592	6.505 7.401 7.099 8.350 8.315 6.485	1.00 14.90 1.00 13.88 1.00 13.08 1.00 11.40 1.00 12.70 1.00 15.62
ATOM ATOM ATOM	1971 1972 1973 1974 1975	O CB CG1 CG2 CD1	ILE A ILE A ILE A ILE A	309 309 309 309 309 310	41.171 38.310 37.346 39.404 36.575	12.112 13.439 14.595 13.887 15.084	6.505 7.401 7.099 8.350 8.315 6.485 6.752	1.00 14.90 1.00 13.88 1.00 13.08 1.00 11.40 1.00 12.70 1.00 15.62 1.00 17.74
MOTA MOTA MOTA MOTA MOTA	1971 1972 1973 1974 1975 1976	O CB CG1 CG2 CD1 N CA	ILE A ILE A ILE A ILE A ILE A LYS A LYS A	309 309 309 309 309 310 310	41.171 38.310 37.346 39.404 36.575 39.475 40.375	12.112 13.439 14.595 13.887 15.084 10.592 9.437	6.505 7.401 7.099 8.350 8.315 6.485	1.00 14.90 1.00 13.88 1.00 13.08 1.00 11.40 1.00 12.70 1.00 15.62
MOTA MOTA MOTA MOTA MOTA MOTA	1971 1972 1973 1974 1975 1976 1977	O CB CG1 CG2 CD1 N CA	ILE A ILE A ILE A ILE A ILE A LYS A LYS A LYS A	309 309 309 309 309 310 310	41.171 38.310 37.346 39.404 36.575 39.475 40.375 41.289	12.112 13.439 14.595 13.887 15.084 10.592 9.437 9.223	6.505 7.401 7.099 8.350 8.315 6.485 6.752 5.559	1.00 14.90 1.00 13.88 1.00 13.08 1.00 11.40 1.00 12.70 1.00 15.62 1.00 17.74 1.00 17.22
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1971 1972 1973 1974 1975 1976 1977 1978 1979	O CB CG1 CG2 CD1 N CA C	ILE A ILE A ILE A ILE A ILE A LYS A LYS A LYS A LYS A	309 309 309 309 309 310 310 310	41.171 38.310 37.346 39.404 36.575 39.475 40.375 41.289 42.532	12.112 13.439 14.595 13.887 15.084 10.592 9.437 9.223 9.061	6.505 7.401 7.099 8.350 8.315 6.485 6.752 5.559 5.715	1.00 14.90 1.00 13.88 1.00 13.08 1.00 11.40 1.00 12.70 1.00 15.62 1.00 17.74 1.00 17.22 1.00 16.87
MOTA MOTA MOTA MOTA MOTA MOTA	1971 1972 1973 1974 1975 1976 1977	O CB CG1 CG2 CD1 N CA	ILE A ILE A ILE A ILE A ILE A LYS A LYS A LYS A	309 309 309 309 309 310 310 310	41.171 38.310 37.346 39.404 36.575 39.475 40.375 41.289	12.112 13.439 14.595 13.887 15.084 10.592 9.437 9.223	6.505 7.401 7.099 8.350 8.315 6.485 6.752 5.559	1.00 14.90 1.00 13.88 1.00 13.08 1.00 11.40 1.00 12.70 1.00 15.62 1.00 17.74 1.00 17.22

ATOM	1981	CG	LYS A	310	39.003	7.953	8.373	1.00 20.85
	1982	CD	LYS A		38.269	6.617	8.432	1.00 22.02
MOTA								
MOTA	1983	CE	LYS A		37.584	6.404	9.757	1.00 25.26
MOTA	1984	NZ	LYS A	310	36.808	5.129	9.752	1.00 26.15
ATOM	1985	N	ALA A	311	40.698	9.211	4.370	1.00 15.56
MOTA	1986	CA	ALA A		41.466	9.007	3.124	1.00 17.77
MOTA	1987	С	ALA A	311	42.549	10.071	2.990	1.00 17.36
ATOM	1988	0	ALA A	311	43.708	9.768	2.578	1.00 20.71
MOTA	1989	CB	ALA A		40.524	9.047	1.908	1.00 14.11
MOTA	1990	N	ALA A	312	42.210	11.309	3.330	1.00 16.63
ATOM	1991	CA	ALA A	312	43.184	12.418	3.235	1.00 15.73
ATOM	1992	C	ALA A		44.247	12.342	4.333	1.00 15.59
MOTA	1993	0	ALA A	312	45.348	12.958	4.207	1.00 13.09
ATOM	1994	CB	ALA A	312	42.449	13.758	3.301	1.00 13.50
ATOM	1995	N	SER A	313	43.950	11.593	5.393	1.00 17.05
					44.867	11.432	6.560	1.00 19.05
MOTA	1996	CA	SER A					
MOTA	1997	С	SER A	313	45.579	10.085	6.593	1.00 19.49
ATOM	1998	0	SER A	313	46.332	9.787	7.568	1.00 21.95
MOTA	1999	CB	SER A		44.075	11.555	7.865	1.00 17.23
			SER A		43.501	12.834	8.003	1.00 23.58
ATOM	2000	OG						
MOTA	2001	N	SER A	314	45.368	9.270	5.570	1.00 20.76
MOTA	2002	CA	SER A	314	45.952	7.909	5.513	1.00 22.73
ATOM	2003	C	SER A		47.436	7.725	5.838	1.00 21.90
					47.825	6.639	6.359	1.00 20.76
ATOM	2004	0	SER A					
ATOM	2005	CB	SER A	314	45.650	7.271	4.150	1.00 22.50
ATOM	2006	OG	SER A	314	46.207	8.032	3.093	1.00 27.94
ATOM	2007	N	THR A		48.285	8.714	5.570	1.00 20.90
					49.732			1.00 23.78
ATOM	2008	CA	THR A			8.523	5.868	
MOTA	2009	C	THR A	315	50.020	8.454	7.361	1.00 25.42
ATOM	2010	0	THR A	315	51.191	8.219	7.784	1.00 26.24
MOTA	2011	CB	THR A		50.616	9.634	5.257	1.00 23.59
ATOM	2012	OG1			50.256	10.901	5.818	1.00 22.73
MOTA	2013	CG2	THR A		50.456	9.668	3.745	1.00 22.59
MOTA	2014	N	GLU A	316	48.994	8.655	8.176	1.00 27.46
MOTA	2015	CA	GLU A	316	49.170	8.589	9.638	1.00 29.81
ATOM	2016	C	GLU A		48.258	7.503	10.201	1.00 30.55
					47.110	7.314	9.710	1.00 29.51
MOTA	2017	0	GLU A					
ATOM	2018	CB	GLU A		48.819	9.931	10.279	1.00 32.51
ATOM	2019	CG	GLU A	316	49.277	10.039	11.725	1.00 36.72
ATOM	2020	CD	GLU A		50.571	10.818	11.879	1.00 36.99
	2021		GLU A		51.456	10.728	11.003	1.00 37.39
ATOM								
MOTA	2022	OE2			50.704	11.522	12.893	1.00 41.14
MOTA	2023	N	LYS A	317	48.736	6.775	11.205	1.00 32.69
ATOM	2024	CA	LYS A	317	47.928	5.702	11.828	1.00 35.09
	2025		LYS A		47.216	6.223	13.071	1.00 33.44
ATOM		C						
MOTA	2026	0	LYS A		47.804	7.005	13.883	1.00 34.13
MOTA	2027	CB	LYS A	317	48.809	4.505	12.202	1.00 38.52
MOTA	2028	CG	LYS A	317	49.980	4.844	13.106	1.00 43.41
	2029	CD	LYS A		50.665	3.588	13.638	1.00 46.99
MOTA								
MOTA	2030	CE	LYS A		51.165	2.686	12.514	1.00 48.65
MOTA	2031	NZ	LYS A	317	51.731	1.410	13.043	1.00 49.49
ATOM	2032	N	PHE A		45.965	5.818	13.245	1.00 31.00
	2033	ĊΑ	PHE A		45.188	6.272	14.408	1.00 30.33
MOTA								
MOTA	2034	С	PHE A		44.683	5.120	15.263	1.00 30.57
MOTA	2035	0	PHE A	318	44.171	4.088	14.732	1.00 29.80
MOTA	2036	СВ	PHE A	318	44.014	7.135	13.944	1.00 28.83
	2037	CG	PHE A		44.436	8.367	13.197	1.00 28.31
MOTA								1.00 27.09
MOTA	2038		PHE A		44.625	8.333	11.817	
ATOM	2039	CD2	PHE A	318	44.686	9.554	13.879	1.00 27.59
ATOM	2040	CE1	PHE A	318	45.060	9.466	11.130	1.00 27.37
ATOM	2041		PHE A		45.122	10.691	13.200	1.00 26.98
ATOM	2042	CZ	PHE A		45.309	10.648	11.826	1.00 27.12
AION	2045	C 2	Enc W	210	30.00	20.040	11.020	

MOTA	2043	N	PRO	Α	319	44.805	5.252	16.591	1.00	30.02
ATOM	2044	CA	PRO	А	319	44.361	4.222	17.535	1 00	30.20
		C								
ATOM	2045.				319	42.864	3.977	17.460		29.88
MOTA	2046	0	PRO	A	319	42.087	4.882	17.040	1.00	29.27
ATOM	2047	CB			319	44.777	4.793	18.890		30.49
ATOM	2048	CG			319	44.667	6.276	18.674		31.99
ATOM .	2049	CD	PRO	Α	319	45.308	6.437	17.309	1.00	30.77
ATOM	2050	N	ASP	Α	320	42.449	2.779	17.860		30.08
ATOM	2051	CA			320					
						41.018	2.389	17.867		29.79
MOTA	2052	С	ASP	Α	320	40.183	3.406	18.652	1.00	28.71
ATOM	2053	0	ASP	Α	320	40.560	3.804	19.804	1.00	27.90
ATOM	2054	CB			320	40.855	1.009			31.81
								18.520		
ATOM	2055	CG	ASP	Α	320	41.545	-0.104	17.740	1.00	34.27
ATOM	2056	OD1	ASP	A	320	41.787	-1.182	18.331	1.00	34.13
ATOM	2057	OD2				41.833	0.092	16.538		35.41
MOTA	2058	N			321	39.067	3.837	18.068	1.00	26.34
ATOM	2059	CA	GLY	Α	321	38.193	4.781	18.745	1.00	24.91
ATOM	2060	С	GLY	А	321	38.439	6.259	18.490	1.00	23.96
MOTA	2061	0	GLY			37.632	7.129	18.941		23.66
MOTA	2062	N	PHE	Α	322	39.519	6.591	17.793	1.00	22.07
ATOM	2063	CA	PHE	Α	322	39.810	8.011	17.507	1.00	20.41
ATOM	2064	C	PHE			38.705	8.670	16.684		20.53
ATOM	2065	0	PHE	A	322	38.157	9.743	17.078		20.75
ATOM	2066	CB	PHE	Α	322	41.126	8.157	16.747	1.00	19.07
ATOM	2067	CG	PHE	Δ	322	41.405	9.567	16.306		19.05
ATOM	2068	CD1				41.701	10.555	17.240	1.00	17.04
ATOM	2069	CD2	PHE	Α	322	41.326	9.918	14.960	1.00	17.20
ATOM	2070	CE1	PHE	Α	322	41.912	11.872	16.840	1.00	18.99
		_				•				
MOTA	2071	CE2	PHE			41.535	11.229	14.552		17.99
MOTA	2072	CZ	PHE	Α	322	41.829	12.210	15.494	1.00	16.28
MOTA	2073	N	TRP	А	323	38.367	8.063	15.552	1.00	20.75
ATOM	2074	CA	TRP			37.330	8.622	14.664		22.37
MOTA	2075	С	TRP	A	323	35.940	8.626	15.273	1.00	23.50
ATOM	2076	Ο.	TRP	Α	323	35.036	9.379	14.804	1.00	22.84
ATOM	2077	CB	TRP			37.322	7.872	13.335		21.45
ATOM	2078	CG	TRP	Α	323	38.643	7.924	12.664	1.00	20.71
MOTA	2079	CD1	TRP	Α	323	39.566	6.921	12.594	1.00	20.50
ATOM	2080	CD2	TRP	Δ	323	39.217	9.049	11.986		20.31
					•					
MOTA	2081	NE1				40.679	7.349	11.913		20.18
MOTA	2082	CE2	TRP	Α	323	40.492	8.651	11.527	1.00	20.95
ATOM	2083	CE3	TRP	Α	323	38.778	10.354	11.722	1.00	20.80
ATOM	2084	CZ2	TRP			41.337				20.49
							9.511	10.816		
ATOM	2085	CZ3	TRP	Α	323	39.618	11.212	11.013	1.00	21.58
MOTA	2086	CH2	TRP	Α	323	40.885	10.784	10.569	1.00	21.15
MOTA	2087	N.	LEU	Α	324	35.734	7.810	16.300	1 00	26.13
	2088		LEU							27.96
ATOM		CA				34.428	7.772	16.983		
ATOM	2089	C	LEU	A	324	34.417	8.877	18.040	1.00	29.09
ATOM	2090	0	LEU	Α	324	33.413	9.044	18.799	1.00	29.23
ATOM	2091	СВ	LEU			34.202		17.642		29.11
							6.408			
MOTA	2092	CG	LEU	A	324	33.910	5.236	16.697	1.00	30.04
ATOM	2093	CD1	LEU	Α	324	33.791	3.948	17.501	1.00	30.31
ATOM	2094		LEU			32.625	5.499	15.924		29.47
ATOM	2095	N	GLY	A	325	35.513	9.634	18.098		29.34
ATOM	2096	CA	GLY	Α	325	35.632	10.728	19.048	1.00	30.68
ATOM	2097	C	GLY			35.794	10.280	20.489		31.19
MOTA	2098	0	GLY			35.687	11.109	21.442		31.53
MOTA	2099	N	GLU	Α	326	36.067	8.995	20.683	1.00	32.22
ATOM	2100	CA	GLU			36.225	8.436	22.042	1.00	34.09
ATOM	2101	C								33.56.
			GLU			37.655	8.482	22.563		
MOTA	2102	0	GLU	Α	326	37.907	8.933	23.720		34.19
ATOM	2103	CB	GLU	A	326	35.728	6.992	22.062	1.00	35.56
ATOM	2104	CG	GLU			34.267	6.847	21.683		38.03
		-0	ں بیات	**	J_ U	JR. 20/	0.047	44.003	1.50	

MOTA	2105	CD	GLU	Α	326	33.855	5.401	21.494	1.00 40.36
MOTA	2106	OE1	GLU	Α	326	32.662	5.162	21.207	1.00 41.84
MOTA	2107.	OE2	GLU	Α	326	34.720	4.506	21.626	1.00 42.10
ATOM	2108	N	GLN			38.602	8.031	21.750	1.00 32.81
MOTA	2109	CA	GLN			40.009	8.017	22.178	1.00 31.36
MOTA	2110	C			327	40.844	9.142	21.608	1.00 30.14
ATOM	2111	0	GLN	Α	327	40.612	9.626	20.458	1.00 28.97
ATOM	2112	CB	GLN	Α	327	40.650	6.667	21.842	1.00 34.41
MOTA	2113	CG	GLN			40.770	5.749	23.060	1.00 38.96
ATOM	2114	CD	GLN			39.443	5.546	23.778	1.00 40.61
MOTA	2115		GLN			39.410	5.223	25.002	1.00 42.73
MOTA	2116	NE2	GLN			38.344	5.714	23.053	1.00 42.75
ATOM	2117	И	LEU			41.814	9.581	22.394	1.00 28.01
MOTA	2118	CA	LEU	A	328	42.695	10.663	21.964	1.00 28.64
MOTA	2119	С	LEU	Α	328	43.889	10.100	21.219	1.00 27.50
ATOM	2120	0	LEU	Α	328	44.207	8.873	21.317	1.00 27.23
MOTA	2121	СВ	LEU			43.177	11.467	23.180	1.00 29.39
ATOM	2122	CG	LEU			43.924	10.735	24.304	1.00 31.09
ATOM	2123		LEU			45.298	10.283	23.831	1.00 31.75
									1.00 31.73
MOTA	2124		LEU			44.074	11.669	25.498	
MOTA	2125	N	VAL			44.539	10.961	20.449	1.00 25.26
ATOM	2126	CA	VAL			45.748	10.583	19.722	1.00 23.64
MOTA	2127	С	VAL	Α	329	46.779	11.593	20.203	1.00 23.76
MOTA	2128	0	VAL	Α	329	46.431	12.786	20.476	1.00 21.96
ATOM	2129	CB	VAL			45.560	10.675	18.194	1.00 23.82
ATOM	2130		VAL			45.100	12.070	17.794	1.00 23.64
ATOM	2131		VAL			46.866	10.317	17.501	1.00 23.70
									1.00 23.70
MOTA	2132	N	CYS			48.025	11.157	20.344	
MOTA	2133	CA	CYS			49.088	12.046	20.830	1.00 24.17
ATOM	2134	С	CYS			50.315	12.060	19.937	1.00 23.87
MOTA	2135	0	CYS	A	330	50.592	11.089	19.165	1.00 24.32
MOTA	2136	CB	CYS	Α	330	49.548	11.633	22.228	1.00 24.93
ATOM	2137	SG	CYS	Α	330	48.353	11.638	23.608	1.00 29.07
ATOM	2138	N	TRP			51.069	13.144	20.047	1.00 22.66
MOTA	2139	CA	TRP			52.306	13.318	19.281	1.00 22.40
	2140	C	TRP			53.333	13.972	20.177	1.00 22.22
ATOM									1.00 22.22
MOTA	2141	0	TRP			52.979	14.698	21.154	
MOTA	2142	CB			331	52.069	14.207	18.064	1.00 21.16
MOTA	2143	CG			331	51.345	13.524	16.959	1.00 19.61
MOTA	2144	CD1	TRP	Α	331	51.868	12.634	16.067	1.00 18.33
MOTA	2145	CD2	TRP	Α	331	49.966	13.684	16.606	1.00 18.42
MOTA	2146	NE1	TRP	Α	331	50.902	12.233	15.177	1.00 17.37
MOTA	2147	CE2	TRP	Α	331	49.721	12.862	15.488	1.00 18.60
ATOM	2148		TRP			48.911	14.446	17.130	1.00 19.20
ATOM	2149		TRP			48.467	12.778	14.874	1.00 17.86
						47.659	14.364	16.521	1.00 19.94
MOTA	2150	CZ3							
MOTA	2151		TRP			47.450	13.535	15.406	1.00 19.08
ATOM	2152	N	GLN			54.598	13.730	19.873	1.00 23.04
MOTA	2153	CA	GLN	Α	332	55.689	14.321	20.648	1.00 25.14
MOTA	2154	С	GLN	Α	332	55.490	15.836	20.594	1.00 23.64
MOTA	2155	0	GLN			55.066	16.397	19.533	1.00 23.11
MOTA	2156	CB	GLN			57.020	13.937	20.015	1.00 27.80
ATOM	2157	ĊG	GLN			58.171	13.877	20.982	1.00 33.30
						59.450	13.445	20.305	1.00 35.55
ATOM	2158	CD	GLN						1.00 36.94
ATOM	2159		GLN			60.060	14.224	19.507	
MOTA	2160		GLN			59.879	12.217	20.579	1.00 36.57
MOTA	2161	N	ALA			55.778	16.506	21.704	1.00 22.79
MOTA	2162	CA	ALA	Α	333	55.618	17.97 7	21.820	1.00 21.04
MOTA	2163	С	ALA	Α	333	55.936	18.759	20.552	1.00 19.77
ATOM	2164	0	ALA			57.076	18.671	19.997	1.00 19.85
ATOM	2165	СВ	ALA			56.475	18.499	22.971	1.00 21.00
MOTA	2166	N	GLY			54.949	19.515	20.083	1.00 17.64
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ATOM	2167	CA	GLY	7	33/	55.123	20.340	18.903	1.00 16.89
MOTA	2168	C	GLY			55.205	19.663	17.548	1.00 17.61
MOTA	2169.	0	GLY	Α	334	55.403	20.370	16.512	1.00 17.50
MOTA	2170	N	THR	Α	335	55.060	18.343	17.490	1.00 16.55
ATOM	2171	CA	THR	Δ	335	55.146	17.648	16.182	1.00 17.58
	2172	C	THR			53.802	17.260	15.557	1.00 16.83
MOTA									
ATOM	2173	0	THR			53.761	16.408	14.618	1.00 17.71
ATOM	2174	CB	THR	Α	335	56.017	16.377	16.275	1.00 17.76
MOTA	2175	OG1	THR	Α	335	55.361	15.401	17.095	1.00 17.56
ATOM	2176	CG2	THR		•	57.373	16.710	16.884	1.00 17.23
MOTA	2177	N	THR			52.707	17.842	16.037	1.00 16.75
ATOM	2178	CA	THR	Α	336	51.373	17.527	15.460	1.00 16.56
ATOM.	2179 ·	С	THR	Α	336	51.473	17.752	13.952	1.00 16.24
ATOM	2180	0	THR	Α	336	51.821	18.868	13.487	1.00 16.30
MOTA	2181	CB	THR	Α	336	50.267	18.437	16.030	1.00 17.05
MOTA	2182	OG1				50.181	18.255	17.451	1.00 17.15
ATOM	2183	CG2	THR			48.917	18.096	15.401	1.00 16.72
MOTA	2184	N	PRO	Α	337	51.182	16.718	13.157	1.00 15.50
ATOM	2185	CA	PRO	Α	337	51.254	16.820	11.699	1.00 14.87
MOTA	2186	С	PRO	Α	337	50.006	17.444	11.082	1.00 14.56
ATOM	2187	0	PRO	Ά	337	49.310	16.800	10.249	1.00 14.49
			PRO			51.448	15.369	11.281	1.00 15.18
ATOM	2188	CB							
MOTA	2189	CG	PRO			50.520	14.657	12.238	1.00 16.05
ATOM	2190	CD	PRO	Α	337	50.784	15.359	13.572	1.00 15.54
ATOM	2191	N	TRP	Α	338	49.713	18.682	11.470	1.00 14.89
ATOM	2192	CA	TRP	А	338	48.535	19.415	10.956	1.00 14.85
ATOM	2193	C	TRP			48.339	19.304	9.445	1.00 14.87
			TRP			47.194	19.048	8.966	1.00 17.13
ATOM	2194	0							
MOTA	2195	СВ	TRP			48.639	20.899	11.313	1.00 13.77
ATOM	2196	CG	TRP	Α	338	48.784	21.176	12.767	1.00 15.11
ATOM	2197	CD1	TRP	Α	338	49.897	21.652	13.411	1.00 14.78
ATOM	2198	CD2	TRP			47.780	21.011	13.771	1.00 14.17
ATOM	2199		TRP			49.641	21.794	14.756	1.00 14.64
ATOM	2200	CE2	TRP			48.348	21.407	15.003	1.00 14.35
ATOM	2201	CE3	TRP			46.451	20.566	13.751	1.00 14.31
ATOM	2202	CZ2	TRP	Α	338	47.635	21.371	16.202	1.00 14.86
MOTA	2203	CZ3	TRP	Α	338	45.744	20.530	14.945	1.00 16.02
ATOM	2204	CH2	TRP	Α	338	46.339	20.932	16.154	1.00 14.77
ATOM	2205	N	ASN			49.414	19.486	8.682	1.00 13.22
	2206		ASN			49.319		7.203	1.00 12.87
ATOM		CA					19.449		
MOTA	2207	С			339	48.674	18.208	6.608	1.00 12.01
MOTA	2208	0	ASN			48.061	18.288	5.508	1.00 13.99
MOTA	2209	ÇВ	ASN	Α	339	50.699	19.649	6.552	1.00 12.61
MOTA	2210	CG	ASN	Α	339	51.576	18.404	6.627	1.00 15.28
ATOM	2211		ASN			52.290	18.174	7.648	1.00 16.29
ATOM	2212		ASN			51.541	17.584	5.578	1.00 12.93
ATOM	2213	N			340	48.774	17.064	7.276	1.00 12.88
ATOM	2214	CA	ILE			48.171	15.831	6.698	1.00 12.98
MOTA	2215	C	ILE	Α	340	46.655	15.864	6.794	1.00 12.80
MOTA	2216	0	ILE	Α	340	45.944	15.237	5.959	1.00 12.80
MOTA	2217	СВ			340	48.667	14.545	7.400	1.00 14.79
								8.833	1.00 14.91
MOTA	2218		ILE			48.142	14.512		
MOTA	2219		ILE			50.194	14.483	7.372	1.00 12.38
MOTA	2220	CD1	ILE	Α	340	48.177	13.142	9.454	1.00 17.42
MOTA	2221	N	PHE	Α	341	46.138	16.577	7.790	1.00 13.19
ATOM	2222		PHE			44.677	16.689	7.972	1.00 13.87
ATOM	2223	C			341	44.143	17.741	7.006	1.00 13.37
			PHE					6.798	1.00 12.72
MOTA	2224	0				44.787	18.812		
ATOM	2225	СВ	PHE			44.354	17.087	9.410	1.00 13.10
MOTA	2226	CG	PHE			44.685	16.027	10.429	1.00 13.55
ATOM	2227	CD1	PHE	Α	341	43.817	14.960	10.654	1.00 13.48
ATOM	2228		PHE			45.861	16.104	11.171	1.00 12.12
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MOTA	2229	CE1	PHE A	341	44.115	13.984	11.607	1.00 13.44
MOTA	2230	CE2	PHE A	341	46.172	15.136	12.127	1.00 14.31
MOTA	2231.	CZ	PHE A		45.298	14.074	12.346	1.00 13.92
ATOM	2232	N	PRO A		42.975	17.484	6.402	1.00 12.78
MOTA	2233	CA	PRO A		42.357	18.413	5.448	1.00 12.17
MOTA	2234	С	PRO A		41.565	19.544	6.100	1.00 12.90
MOTA	2235	0	PRO A		41.168	19.465	7.309	1.00 12.52
MOTA	2236	CB	PRO A		41.447	17.502	4.638	1.00 10.18
MOTA	2237	CG	PRO A		40.920	16.570	5.714	1.00 11.48
ATOM	2238	CD	PRO A		42.180	16.244	6.523	1.00 12.10
ATOM	2239	N	VAL A		41.342	20.609	5.342	1.00 12.27
MOTA	2240	CA	VAL A		40.528	21.712	5.851	1.00 10.51
MOTA	2241	C	VAL A		39.101	21.281	5.521	1.00 12.41
MOTA	2242 2243	O CB	VAL A		38.878 40.838	20.401 23.054	4.632 5.143	1.00 10.45 1.00 10.23
ATOM ATOM	2243		VAL A		40.838	23.507	5.488	1.00 10.23
ATOM	2244		VAL A		40.672	22.914	3.636	1.00 8.08
ATOM	2246	N	ILE A		38.132	21.848	6.224	1.00 13.49
ATOM	2247	CA	ILE A		36.725	21.507	5.991	1.00 13.17
ATOM	2248	C	ILE A		35.989	22.789	5.664	1.00 13.33
MOTA	2249	ō	ILE A		36.067	23.795	6.427	1.00 13.12
MOTA	2250	CB	ILE A		36.099	20.859	7.246	1.00 14.77
ATOM	2251	CG1			36.776	19.512	7.517	1.00 14.50
ATOM	2252	CG2	ILE A	344	34.585	20.702	7.060	1.00 13.14
ATOM	2253	CD1	ILE A	344	36.374	18.875	8.825	1.00 17.73
MOTA	2254	N	SER A	345	35.292	22.794	4.537	1.00 12.41
MOTA	2255	CA	SER A	345	34.547	23.982	4.136	1.00 13.41
MOTA	2256	С	SER A		33.051	23.723	4.172	1.00 14.94
ATOM	2257	0	SER A		32.555	22.641	3.721	1.00 14.55
MOTA	2258	CB	SER A		34.967	24.430	2.728	1.00 14.23
MOTA	2259	OG	SER A		36.329	24.834	2.703	1.00 13.57
MOTA	2260	N	LEU A		32.320	24.682	4.725	
ATOM	2261	CA	LEU A		30.859	24.594	4.796	1.00 14.08
MOTA	2262	C	LEU A		30.320	25.772 26.956	4.003 4.286	1.00 13.86 1.00 13.52
MOTA	2263 2264	O CB	LEU A		30.681 30.383	24.674	6.252	1.00 15.83
MOTA MOTA	2265	CG	LEU A		30.333	23.372	7.051	1.00 13.03
ATOM	2266		LEU A		31.455	22.492	6.875	1.00 17.74
ATOM	2267		LEU A		30.028	23.711	8.521	1.00 19.69
MOTA	2268	N	TYR A		29.496	25.485	3.000	1.00 13.48
ATOM	2269	CA	TYR A		28.894	26.543	2.176	1.00 13.76
ATOM	2270	С	TYR A	347	27.525	26.864	2.745	1.00 14.58
ATOM	2271	0	TYR A	347	26.676	25.948	2.979	1.00 13.16
MOTA	2272	СВ	TYR A	347	28.757	26.101	0.716	1.00 14.82
ATOM	2273	CG	TYR A		30.066	26.051	-0.034	1.00 15.10
ATOM	2274		TYR A		31.022	25.074	0.252	1.00 13.97
MOTA	2275		TYR A		30.349	26.977	-1.038	1.00 13.98
ATOM	2276		TYR A		32.228	25.018	-0.447	1.00 14.47
MOTA	2277		TYR A		31.556	26.930	-1.746	1.00 15.69
ATOM	2278	CZ	TYR A		32.487	25.949	-1.445 -2.141	1.00 15.09 1.00 16.72
ATOM	2279 2280	OH	TYR A LEU A		33.672	25.895 28.145	2.971	1.00 18.72
MOTA MOTA	2280	CA U	LEU A		27.288 26.018	28.593	3.545	1.00 15.88
ATOM	2282	CA	LEU A		25.246	29.445	2.559	1.00 10.70
ATOM	2283	0	LEU A			30.183	1.722	1.00 16.05
ATOM	2284	СВ	LEU A		26.292	29.401	4.814	1.00 15.57
ATOM	2285	CG	LEU A		27.019	28.620	5.908	1.00 17.10
ATOM	2286		LEU A		27.518	29.565	6.985	1.00 15.71
ATOM	2287		LEU A		26.078	27.580	6.495	1.00 16.92
ATOM	2288	N	MET A		23.922	29.352	2.617	1.00 19.68
MOTA	2289	CA	MET A		23.073	30.167	1.734	1.00 22.78
MOTA	2290	С	MET A	349	23.384	31.629	2.024	1.00 22.03
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ATOM	2291	0	MET	Α	349	23.478	32.049	3.222	1.00 20.70
ATOM	2292	CB	MET	Α	349	21.594	29.897	2.008	1.00 25.40
ATOM	2293	CG	MET			20.931	28.954	1.012	1.00 31.18
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ATOM	2294	SD	MET			19.139	28.833	1.272	1.00 37.43
ATOM	2295	CE	MET	А	349	18.697	30.583	1.318	1.00 32.73
ATOM	2296	N	GLY	Α	350	23.573	32.414	0.972	1.00 20.81
MOTA	2297	CA	GLY			23.857	33.824	1.167	1.00 23.50
MOTA	2298	С	GLY			22.565	34.612	1.280	1.00 24.26
ATOM	2299	0	GLY	Α	350	21.450	34.042	1.091	1.00 23.13
MOTA	2300	N	GLU	Α	351	22.662	35.899	1.591	1.00 27.25
ATOM	2301	CA	GLU	А	351	21.448	36.734	1.698	1.00 32.00
-		C	GLU			20.870	36.948	0.306	1.00 33.92
MOTA	2302		-						
ATOM	2303	0	GLU			19.620	37.066	0.125	1.00 34.42
ATOM	2304	CB	GLU	Α	351	21.774	38.081	2.340	1.00 32.31
ATOM	2305	CG	GLU	Α	351	22.012	37.996	3.831	1.00 34.92
ATOM	2306	CD	GLU	А	351	21.916	39.346	4.503	1.00 35.55
ATOM	2307		GLU			22.819	40.187	4.293	1.00 36.64
ATOM	2308		GLU			20.927	39.567	5.233	1.00 36.29
MOTA	2309	N	VAL	Α	352	21.753	37.007	-0.684	1.00 36.98
MOTA	2310	CA	VAL	Α	352	21.327	37.181	-2.082	1.00 38.72
ATOM	2311	С	VAL	Α	352	20.944	35.809	-2.629	1.00 40.47
ATOM	2312	ō	VAL			21.689	34.799	-2.426	1.00 39.68
MOTA	2313	CB	VAL			22.456	37.767	-2.939	1.00 38.31
MOTA	2314	CG1	VAL	Α	352	21.999	37.892	-4.382	1.00 38.33
ATOM	2315	CG2	VAL	Α	352	22.866	39.123	-2.391	1.00 37.93
MOTA	2316	N	THR	А	353	19.806	35.747	-3.314	1.00 42.33
ATOM	2317	CA	THR			19.300	34.476	-3.882	1.00 43.97
MOTA	2318	С	THR			20.254	33.832	-4.877	1.00 43.18
MOTA	2319	0	THR	Α	353	20.941	34.536	-5.688	1.00 42.65
MOTA	2320	CB	THR	Α	353	17.929	34.672	-4.578	1.00 45.29
ATOM	2321	OG1				18.018	35.743	-5.526	1.00 46.63
	2322		THR			16.849	34.988	-3.551	1.00 46.31
MOTA									
MOTA	2323	N	ASN			20.307	32.507	-4.839	1.00 42.20
MOTA	2324	CA	ASN	Α	354	21.183	31.741	-5.742	1.00 43.39
ATOM	2325	С	ASN	A	354	22.641	32.166	-5.611	1.00 41.22
ATOM	2326	0	ASN			23.444	32.078	-6.584	1.00 43.04
	2327	СВ	ASN			20.698	31.887	-7.187	1.00 45.64
ATOM									
MOTA	2328	CG	ASN		_	19.467	31.036	-7.474	1.00 47.44
ATOM	2329	OD1	ASN	Α	354	18.824	31.163	-8.562	1.00 48.61
MOTA	2330	ND2	ASN	Α	354	19.121	30.159	-6.534	1.00 47.73
MOTA	2331	N	GLN	А	355	22.999	32.621	-4.419	1.00 37.62
ATOM	2332	CA	GLN			24.371	33.042	-4.128	1.00 34.85
									1.00 34.03
ATOM	2333	С	GLN			24.737	32.475	-2.764	
ATOM	2334	0	GLN	А	355	23.863	32.388	-1.846	1.00 31.25
ATOM	2335	CB	GLN	Α	355	24.459	34.563	-4.105	1.00 35.77
ATOM	2336	CG	GLN	Α	355	25.834	35.089	-3.797	1.00 38.04
ATOM	2337	CD	GLN			25.909	36.590	-3.915	1.00 39.05
								-4.992	1.00 40.57
MOTA	2338		GLN			25.586	37.171		
ATOM	2339	NE2	GLN	А	355	26.331	37.249	-2.844	1.00 39.68
ATOM	2340	N	SER	Α	356	25.989	32.071	-2.597	1.00 29.33
ATOM	2341	CA	SER	Α	356	26.419	31.514	-1.304	1.00 25.60
ATOM	2342	С	SER			27.850	31.897	-0.981	1.00 22.66
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ATOM	2343	Ö	SER			28.580	32.481	-1.833	1.00 21.99
ATOM	2344	CB	SER			26.313	29.991	-1.318	1.00 25.71
MOTA	2345	OG	SER	Α	356	27.449	29.425	-1.945	1.00 24.59
MOTA	2346	N	PHE			28.267	31.583	0.239	1.00 20.53
ATOM	2347	CA	PHE			29.639	31.865	0.676	1.00 17.95
								1.437	1.00 17.15
ATOM	2348	C	PHE			30.104	30.643		
MOTA	2349	0	PHE			29.279	29.750	1.784	1.00 17.21
MOTA	2350	CB	PHE	A	357	29.687	33.126	1.550	1.00 17.62
ATOM	2351	CG	PHE	Α	357	28.926	33.017	2.850	1.00 17.61
ATOM	2352		PHE			29.571	32.625	4.018	1.00 15.09

ATOM	2353	CD2	PHE	Α	357	2	27.577	7	33.357	2.912	1.00	16.90
ATOM	2354	CE1	PHE	А	357	2	8.887	7	32.577	5.229	1.00	14.87
MOTA	2355	CE2	PHE	A	357	2	26.881	1	33.312	4.120	1.00	15.64
MOTA	2356	CZ	PHE	Α	357	2	27.538	В	32.924	5.280	1.00	16.14
MOTA	2357	N	ARG	Α	358	3	31.397	7	30.545	1.687	1.00	16.29
ATOM	2358	CA	ARG	Α	358	3	31.891	l	29.383	2.412	1.00	14.04
MOTA	2359	С	ARG	Α	358	3	32.642	2	29.755	3.664	1.00	14.59
ATOM	2360	0	ARG			3	33.237	7	30.869	3.785	1.00	13.01
MOTA	2361	CB	ARG	A	358	3	32.784	4	28.525	1.516	1.00	14.11
MOTA	2362	CG	ARG	Α	358	3	34.084	4	29.172	1.102	1.00	13.28
ATOM	2363	CD	ARG	Α	358	3	34.809	9	28.275	0.121	1.00	13.06
ATOM	2364	NE	ARG	A	358	3	36.090	0	28.831	-0.291	1.00	14.39
ATOM	2365	CZ	ARG	А	358	3	36.723	3	28.489	-1.409	1.00	14.92
ATOM	2366	NH1	ARG	Α	358	3	36.188	В	27.591	-2.232	1.00	13.71
ATOM	2367	NH2	ARG	Α	358	3	37.888	8	29.045	-1.701	1.00	12.88
ATOM	2368	N	ILE	Α	359	3	32.612	2	28.819	4.596	1.00	14.51
ATOM	2369	CA	ILE	Α	359	3	33.268	8	28.935	5.891	1.00	16.36
ATOM	2370	С	ILE				34.242	2	27.762	5.913	1.00	15.41
MOTA	2371	0	ILE	Α	359	3	33.836	6	26.583	5.675	1.00	15.49
ATOM	2372	CB	ILE	Α	359	3	32.197	7	28.824	7.001	1.00	
MOTA	2373	CG1	ILE	Α	359	;	31.543	3	30.190	7.198	1.00	19.68
MOTA	2374	CG2	ILE	Α	359		32.76	6	28.260	8.255	1.00	20.12
MOTA	2375	CD1	ILE	A	359	3	32.51	5	31.288	7.500	1.00	22.40
MOTA	2376	N	THR	A	360	3	35.513	3	28.046	6.162	1.00	13.01
MOTA	2377	CA	THR	A	360	:	36.53	1	26.983	6.167	1.00	14.32
MOTA	2378	С	THR	Α	360		37.30	7	26.894	7.470	1.00	14.04
MOTA	2379 .	0	THR	Α	360		37.892	2	27.913	7.938	1.00	13.82
MOTA	2380	CB	THR	Α	360	3	37.53	6	27.202	5.021	1.00	
ATOM	2381	OG1	THR	Α	360		36.82	8	27.286	3.774		15.69
MOTA	2382	CG2	THR	Α	360		38.53	2	26.053	4.964		15.11
MOTA	2383	N	ILE	Α	361		37.33	1	25.709	8.074		13.79
ATOM	2384	CA	ILE	Α	361		38.09	1	25.524	9.330	1.00	
MOTA	2385	С	ILE	А	361		39.24		24.548	9.122	1.00	
MOTA	2386	0	ILE				39.23		23.717	8.160		16.37
MOTA	2387	CB	ILE				37.20		24.982	10.476	1.00	
MOTA	2388	CG1	ILE	Α	361		36.60		23.632	10.077		
MOTA	2389	CG2	ILE				36.12		25.999	10.830		18.95
MOTA	2390	-	ILE				35.89		22.937	11.208		18.19
MOTA	2391	N	LEU				40.23		24.614	9.998	1.00	
MOTA	2392	CA	LEU				41.37		23.710	9.876		18.92
MOTA	2393	С	LEU				41.41		22.659	10.983		17.87
MOTA	2394	0	LEU				40.53		22.654	11.912		17.21
MOTA	2395	CB			362		42.67	_	24.525	9.837	1.00	
MOTA	2396	CG	LEU				42.68		25.974	10.320	1.00	
ATOM	2397		LEU				42.94		25.992	11.802	1.00 1.00	
MOTA	2398		LEU				43.78		26.751	9.623	1.00	
MOTA	2399	N			363		42.38		21.729	10.910 11.925	1.00	
MOTA	2400	CA			363		42.50		20.681		1.00	
MOTA	2401	C			363		42.62		21.325	13.303	1.00	
MOTA	2402	0			363		42.23		20.710	14.339 11.534	1.00	
ATOM	2403	CB			363		43.80		19.971	10.076	1.00	
ATOM	2404	CG			363		43.90		20.202	9.903	1.00	
MOTA	2405	CD	-		363		43.45		21.616	13.337	1.00	
ATOM	2406	N			364		43.17		22.539	14.608	1.00	
ATOM	2407	CA			364		43.35		23.271	15.254	1.00	
MOTA	2408	C			364		42.01		23.557 23.895	16.467	1.00	
ATOM	2409	0			364 364		41.95 44.11		24.585	14.392	1.00	
ATOM	2410	CB			364		44.11 45.63		24.363	14.304	1.00	
MOTA	2411	CG			364		45.63 46.14		24.449	12.919	1.00	
ATOM	2412	CD OF1	GLN				40.14 47.37		24.079	12.625	1.00	
ATOM	2413		GLN				47.37 45.24		23.621	12.056	1.00	8.04
ATOM	2414	MEZ	GTIA	Α.	J U 4		4	J	2J.V2I			

MOTA	2415	N	GLN	Α	365	40.939	23.446	14.478	1.00 13.30
MOTA	2416	CA	GLN	Α	365	39.580	23.657	15.023	1.00 14.36
MOTA	2417	С	GLN			38.873	22.341	15.339	1.00 14.57
						38.312	22.175	16.457	1.00 14.57
MOTA	2418	0	GLN						
ATOM	2419	CB	GLN			38.691	24.452	14.056	1.00 14.03
MOTA	2420	CG	GLN	Α	365	38.816	25.962	14.167	1.00 15.23
MOTA	2421	CD	GLN	Α	365	40.073	26.489	13.515	1.00 15.81
MOTA	2422	OE1	GLN	Α	365	40.290	26.292	12.282	1.00 15.51
ATOM	2423	NE2				40.917	27.158	14.295	1.00 15.82
ATOM	2424	N			366	38.873	21.392	14.406	1.00 14.93
MOTA	2425	CA			366	38.149	20.128	14.673	1.00 15.12
ATOM	2426	С	TYR			38.914		15.447	1.00 15.66
MOTA	2427	0	TYR	Α	366	38.378	17.930	15.703	1.00 17.42
MOTA	2428	CB	TYR	Α	366	37.557	19.567	13.371	1.00 14.28
MOTA	2429	CG	TYR	A	366	38.541	19.107	12.322	1.00 13.05
MOTA	2430	CD1	TYR	Α	366	39.228	17.907	12.467	1.00 13.67
ATOM	2431	CD2				38.721	19.835	11.145	1.00 13.44
ATOM	2432	CE1				40.062	17.431	11.463	1.00 12.91
						39.555	19.369	10.128	1.00 12.63
MOTA	2433	CE2							
MOTA	2434	CZ			366	40.218	18.163	10.294	1.00 13.86
MOTA	2435	OH	TYR			41.008	17.669	9.287	1.00 12.42
MOTA	2436	N	LEU	Α	367	40.144	19.367	15.835	1.00 16.84
MOTA	2437	CA	LEU	Α	367	40.966	18.450	16.660	1.00 16.98
ATOM	2438	С	LEU	Α	367	40.996	19.161	18.017	1.00 17.50
ATOM	2439	0	LEU	А	367	41.662	20.224	18.172	1.00 16.40
ATOM	2440	CB	LEU			42.382	18.324	16.088	1.00 17.44
ATOM	2441	CG	LEU			42.764	16.991	15.429	1.00 17.44
MOTA	2442		LEU			41.681	16.534	14.482	1.00 17.60
MOTA	2443		LEU			44.091	17.143	14.700	1.00 17.38
MOTA	2444	N	ARG	A	368	40.270	18.624	18.990	1.00 17.06
MOTA	2445	CA	ARG	Α	368	40.192	19.253	20.326	1.00 17.22
ATOM	2446	С	ARG	Α	368	41.341	18.874	21.243	1.00 16.52
ATOM	2447	0	ARG	A	368	41.554	17.662	21.538	1.00 16.19
MOTA	2448	CB	ARG			38.879	18.871	21.009	1.00 16.02
MOTA	2449	CG	ARG			38.050	20.055	21.444	1.00 19.09
ATOM	2450	CD	ARG			37.415	19.811	22.792	1.00 17.88
MOTA	2451	NE	ARG			36.840	18.474	22.906	1.00 17.20
MOTA	2452	CZ	ARG		_	36.775	17.806	24.053	1.00 18.65
ATOM	2453		ARG			37.247	18.361	25.164	1.00 18.77
ATOM	2454	NH2	ARG			36.258	16.584	24.095	1.00 17.53
ATOM	2455	N	PRO	Α	369	42.100	19.867	21.722	1.00 17.88
ATOM	2456	CA	PRO	Α	369	43.220	19.558	22.615	1.00 19.69
ATOM	2457	С	PRO	Α	369	42.744	19.067	23.969	1.00 22.16
ATOM	2458	0	PRO			41.786	19.645	24.575	1.00 20.49
MOTA	2459	СВ	PRO			43.983	20.883	22.700	1.00 20.03
		CG	PRO			42.932	21.911	22.429	1.00 19.96
ATOM	2460							21.320	1.00 17.42
MOTA	2461	CD	PRO			42.122	21.285		
MOTA	2462	N	VAL			43.376	18.001	24.444	1.00 23.75
MOTA	2463	CA	VAL	Α	370	43.040	17.399	25.747	1.00 27.84
MOTA	2464	С	VAL	Α	370	44.332	16.921	26.394	1.00 30.26
MOTA	2465	0	VAL	Α	370	45.321	16.577	25.682	1.00 30.79
ATOM	2466	CB	VAL	Α	370	42.093	16.197	25.577	1.00 26.52
ATOM	2467		VAL	Α	370	40.771	16.654	24.989	1.00 26.57
MOTA	2468		VAL			42.737	15.160	24.669	1.00 26.53
	2469	N	GLU			44.361	16.891	27.719	1.00 35.50
MOTA									1.00 40.60
ATOM	2470	CA	GLU			45.574	16.450	28.426	
MOTA	2471	C	GLU			45.800	14.963	28.235	1.00 42.42
ATOM	2472	0	GLU			44.832	14.138	28.321	1.00 41.89
MOTA	2473	CB	GLU			45.472	16.758	29.921	1.00 43.12
MOTA	2474	CG	GLU	A	371	46.603	17.634	30.443	1.00 47.33
ATOM	2475	CD	GLU	Α	371	47.954	17.245	29.864	1.00 49.98
ATOM	2476		GLU	Α	371	48.264	16.036	29.818	1.00 51.63

ATOM	2477	OE2	GLU	А	371	48.710	18.151	29.456	1.00 51.00
ATOM	2478	N	ASP			47.046	14.596	27.960	1.00 45.77
ATOM	2479	CA	ASP			47.396	13.182	27.774	1.00 49.75
ATOM	2480	C			372	46.889	12.468	29.014	1.00 52.41
ATOM	2481	ō	ASP			47.090	12.966	30.165	1.00 52.32
	2482	СВ			372	48.913	13.015	27.665	1.00 52.32
MOTA								27.333	
MOTA	2483	CG	ASP			49.323	11.587		1.00 51.15
ATOM	2484		ASP			50.541	11.323	27.246	1.00 51.32
ATOM	2485		ASP			48.429	10.729	27.156	1.00 50.76
MOTA	2486	N	VAL			46.217	11.340	28.819	1.00 55.35
ATOM	2487	CA	VAL			45.688	10.570	29.956	1.00 58.73
MOTA	2488	С	VAL			46.850	10.213	30.896	1.00 60.04
MOTA.	2489·	0	VAL			47.465	9.105	30.817	1.00 60.06
MOTA	2490	CB	VAL			44.901	9.313	29.433	1.00 59.43
MOTA	2491		VAL			45.292	8.044	30.176	1.00 59.64
MOTA	2492	CG2	VAL	Α	373	43.402	9.556	29.597	1.00 59.89
MOTA	2493	N	ALA	Α	374	47.187	11.169	31.759	1.00 61.58
ATOM	2494	CA	ALA	Α	374	48.277	11.020	32.755	1.00 61.52
MOTA	2495	С	ALA	Α	374	49.709	11.205	32.233	1.00 61.38
MOTA	2496	0	ALA	Α	374	50.104	10.633	31.169	1.00 60.95
MOTA	2497	CB	ALA	Α	374	48.155	9.668	33.455	1.00 62.66
ATOM	2498	N	THR	Α	375	50.477	12.002	32.977	1.00 61.03
ATOM	2499	CA	THR			51.919	12.320	32.715	1.00 60.30
ATOM	2500	С	THR	Α	375	52.401	12.358	31.269	1.00 58.41
ATOM	2501	ō	THR			52.361	11.308	30.555	1.00 59.21
ATOM	2502	СВ	THR			52.838	11.327	33.455	1.00 61.35
ATOM	2503	OG1				52.302	11.049	34.756	1.00 62.26
ATOM	2504	CG2				54.237	11.912	33.599	1.00 61.47
MOTA	2505	N	SER			52.892	13.520	30.833	1.00 55.18
MOTA	2506	CA			376	53.407	13.683	29.445	1.00 51.40
MOTA	2507	C	SER			53.538	15.132	28.981	1.00 31.40
	2508	o			376	52.887	16.067	29.540	1.00 48.19
MOTA	2509				376	52.502	12.943	28.456	1.00 40.19
MOTA		CB				52.880	13.193	27.115	1.00 51.90
MOTA	2510	OG			376			27.113	1.00 31.94
MOTA	2511	N	GLN			54.373	15.333		
ATOM	2512	CA	GLN			54.576	16.664	27.367	1.00 41.28
MOTA	2513	C	GLN			54.106	16.580	25.923	1.00 37.22
MOTA	2514	0	GLN			54.380	17.489	25.081	1.00 35.23
ATOM	2515	CB	GLN			56.048	17.062	27.425	1.00 43.59
MOTA	2516	CG	GLN			56.468	17.585	28.789	1.00 46.22
ATOM	2517	CD	GLN			57.955	17.831	28.886	1.00 47.12
MOTA	2518	OE1				58.710	17.710	27.867	1.00 48.44
MOTA	2519	NE2	GLN			58.414	18.177	30.081	1.00 48.23
ATOM	2520	N	ASP			53.399	15.499	25.618	1.00 31.89
ATOM '	2521	CA	ASP			52.866	15.289	24.263	1.00 28.31
ATOM	2522	C	ASP			51.663	16.183	24.034	1.00 25.36
MOTA	2523	0	ASP			50.958	16.590	25.004	1.00 22.58
MOTA	2524	CB	ASP	Α	378	52.422	13.835	24.072	1.00 28.64
MOTA	2525	CG	ASP	Α	378	53.582	12.867	23.998	1.00 29.19
MOTA	2526		ASP			54.746	13.316	23.948	1.00 30.91
ATOM	2527	OD2	ASP	Α	378	53.323	11.647	23.981	1.00 30.50
MOTA	2528	N	ASP	Α	379	51.415	16.513	22.776	1.00 23.06
MOTA	2529	СA	ASP	Α	379	50.236	17.317	22.436	1.00 22.51
ATOM	2530	C	ASP	Α	379	49.220	16.294	21.964	1.00 21.46
MOTA	2531	0	ASP			49.436	15.581	20.945	1.00 19.87
ATOM	2532	CB			379	50.570	18.335	21.346	1.00 21.72
MOTA	2533	CG			379	51.557	19.377	21.829	1.00 23.29
MOTA	2534		ASP			51.434	19.786	23.005	1.00 23.00
MOTA	2535		ASP			52.446	19.789	21.052	1.00 23.50
ATOM	2536	N			380	48.128		22.706	1.00 20.99
ATOM	2537	CA			380	47.082	15.201	22.393	1.00 20.40
MOTA	2538	C			380	45.769	15.865	22.013	1.00 19.94
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ATOM	2539	0	CYS A	380	45.489	17.038	22.417	1.00 18.77
MOTA	2540	CB	CYS A	380	46.867	14.292	23.596	1.00 23.14
MOTA	2541.	SG	CYS A	380	48.368	13.550	24.327	1.00 25.25
MOTA	2542	N	TYR A		44.947	15.140	21.255	1.00 18.49
MOTA	2543	CA	TYR A		43.656	15.681	20.785	1.00 17.31
MOTA	2544	С	TYR A		42.595	14.610	20.602	1.00 17.45
MOTA	2545	0	TYR A		42.890	13.376	20.532	1.00 16.46
MOTA	2546	СВ	TYR A		43.833	16.370	19.427	1.00 15.47
ATOM	2547	CG	TYR A		45.034	17.275	19.314	1.00 14.93
MOTA	2548	CD1	TYR A		44.899	18.659	19.408	1.00 14.20
MOTA	2549	CD2	TYR A		46.311	16.746	19.118	1.00 14.17
MOTA	2550	CE1	TYR A		46.009	19.499	19.307	1.00 14.66
MOTA	2551	CE2	TYR A		47.431	17.576	19.021	1.00 15.73
MOTA	2552	CZ	TYR A		47.272	18.952	19.113	1.00 16.02 1.00 15.32
MOTA	2553 2554	OH	TYR A		48.369 41.356	19.785 15.066	18.994 20.506	1.00 13.32
MOTA MOTA	2555	N CA	LYS F		40.218	14.174	20.308	1.00 20.26
ATOM	2556	CA	LYS A		39.555	14.695	18.981	1.00 20.20
MOTA	2557	0	LYS A		39.575	15.941	18.704	1.00 19.65
ATOM	2558	CB	LYS A		39.221	14.204	21.404	1.00 21.74
ATOM	2559	CG	LYS A		39.632	13.348	22.585	1.00 25.42
ATOM	2560	CD	LYS A		38.509	13.266	23.602	1.00 27.59
ATOM	2561	CE	LYS F		38.878	12.342	24.759	1.00 29.84
MOTA	2562	NZ	LYS A		37.779	12.246	25.761	1.00 31.22
MOTA	2563	N	PHE A		38.994	13.786	18.192	1.00 18.55
MOTA	2564	CA	PHE A	383	38.298	14.165	16.942	1.00 16.97
MOTA	2565	С	PHE A	383	36.992	14.823	17.375	1.00 16.22
ATOM	2566	0	PHE A	383	36.079	14.138	17.908	1.00 13.73
MOTA	2567	CB	PHE A	383	38.026	12.907	16.110	1.00 16.57
MOTA	2568	CG	PHE A	383	37.447	13.182	14.750	1.00 16.49
MOTA	2569	CD1			38.052	14.091	13.890	1.00 14.48
MOTA	2570	CD2	PHE A		36.319	12.489	14.308	1.00 15.06
MOTA	2571	CE1	PHE A		37.542	14.306	12.606	1.00 16.02
MOTA	2572	CE2	PHE A		35.807	12.696	13.029	1.00 15.64
MOTA	2573	CZ	PHE A		36.419	13.603	12.176	1.00 15.10
MOTA	2574	N	ALA A		36.885	16.134	17.173	1.00 16.28
ATOM	2575	CA	ALA A		35.675	16.893	17.586	1.00 15.54 1.00 15.46
ATOM ATOM	2576 2577	C O	ALA A		34.549, 33.768	16.931 17.931	16.559 16.487	1.00 15.40
ATOM	2578	СВ	ALA A		36.061	18.316	17.987	1.00 14.96
ATOM	2579	N	ILE A		34.451	15.888	15.745	1.00 14.66
ATOM	2580	CA	ILE A		33.356	15.792	14.763	1.00 13.45
ATOM	2581	C	ILE A		32.651	14.487	15.093	1.00 14.39
ATOM	2582	ŏ	ILE A		33.303	13.410	15.179	1.00 12.37
ATOM	2583	CB	ILE A		33.862	15.724	13.315	1.00 12.54
ATOM	2584	CG1			34.696	16.959	12.988	1.00 13.08
ATOM	2585	CG2	ILE A		32.675	15.655	12.367	1.00 12.56
MOTA	2586	CD1	ILE A		35.178	17.003	11.549	1.00 10.74
ATOM	2587	N	SER A	386	31.343	14.543	15.297	1.00 14.95
MOTA	2588	CA	SER A	386	30.605	13.319	15.637	1.00 16.99
MOTA	2589	С	SER A		29.275	13.221	14.918	1.00 17.48
MOTA	2590	0	SER A		28.795	14.207	14.279	1.00 18.09
MOTA	2591	СВ	SER A		30.385	13.240	17.151	1.00 16.69
ATOM	2592	OG	SER A		29.630	14.345	17.616	1.00 16.81
MOTA	2593	N	GLN A		28.673	12.044	15.016	1.00 19.86
MOTA	2594	CA	GLN A		27.384	11.748	14.376	1.00 23.09
MOTA	2595	С	GLN A		26.209	12.317	15.160	1.00 22.61
MOTA	2596	0	GLN A		26.221	12.363	16.427	1.00 22.90
ATOM	2597 2598	CB	GLN A		27.222	10.234 9.795	14.247 13.411	1.00 24.53
ATOM ATOM	2598 2599	CG CD	GLN A		26.035 25.971	8.286	13.411	1.00 28.94
MOTA	2600	OE1			27.013	7.619	12.999	1.00 30.39
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MOTA	2601	NE2	GLN	Α	387	24.782	7.721	13.441	1.00 32.07
ATOM	2602	N	SER	А	388	25.186	12.743	14.434	1.00 21.60
MOTA	2603	CA			388	23.981	13.306	15.055	
									1.00 21.59
ATOM	2604	С			388	22.728	12.711	14.429	1.00 22.68
ATOM	2605	0	SER	'A	388	22.707	12.380	13.203	1.00 23.08
ATOM	2606	СВ			388'	23.959	14.824	14.871	1.00 19.88
		•							
MOTA	2607	OG	SER	Α	388	22.661	15.342	15.112	1.00 19.18
ATOM	2608	N	SER	Α	389	21.681	12.551	15.227	1.00 23.51
ATOM	2609	CA			389	20.405	12.024	14.690	1.00 24.44
MOTA	2610	C			389	19.391	13.167	14.708	1.00 23.83
MOTA	2611	0	SER	Α	389	18.181	12.973	14.385	1.00 23.81
ATOM	2612	CB	SER	А	389	19.902	10.847	15.534	1.00 25.63
ATOM	2613				389	19.681	11.235	16.881	
		OG							1.00 27.65
MOTA	2614	N	THR	Α	390	19.861	14.360	15.066	1.00 22.66
ATOM	2615	CA	THR	Α	390	18.984	15.553	15.127	1.00 22.60
MOTA	2616	С	THR	Δ	390	19.471	16.709	14.260	1.00 21.12
MOTA	2617	0			390	19.272	17.910	14.608	1.00 21.35
MOTA	2618	CB	THR	Α	390	18.825	16.052	16.577	1.00 23.02
MOTA	2619	OG1	THR	Α	390	20.117	16.288	17.150	1.00 24.55
ATOM	2620	CG2			390	18.079	15.010	17.413	1.00 23.83
MOTA	2621	N			391	20.093	16.381	13.136	1.00 19.75
ATOM	2622	CA	GLY	Α	391	20.573	17.410	12.237	1.00 16.88
ATOM	2623	С	GLY	Α	391	21.982	17.891	12.526	1.00 17.24
ATOM	2624	Ō			391	22.672		/13.472	1.00 16.27
			-						
ATOM	2625	N			392	22.427	18.851	11.730	1.00 14.99
ATOM	2626	CA	THR	Α	392	23.773	19.423	11.880	1.00 14.81
ATOM	2627	С	THR	Α	392	23.841	20.514	12.938	1.00 14.47
ATOM	2628	ō			392	22.949	21.409	13.012	
							•		1.00 16.11
MOTA	2629	CB	THR	Α	392	24.266	20.062	10.564	1.00 12.95
ATOM	2630	OG1	THR	Α	392	24.494	19.043	9.588	1.00 14.51
ATOM	2631	CG2	THR	Δ	392	25.572	20.839	10.800	1.00 14.09
MOTA	2632	N	VAL			24.857	20.458	13.779	1.00 13.06
MOTA	2633	CA	VAL	Α	393	25.027	21.534	14.746	1.00 15.07
ATOM	2634	С	VAL	Α	393	26.462	22.033	14.684	1.00 15.47
ATOM	2635	o	VAL			27.450	21.265	14.908	1.00 16.85
MOTA	2636	СВ			393	24.619	21.128	16.201	1.00 16.35
MOTA	2637	CGI	VAL	Α	393	24.559	19.624	16.348	1.00 15.06
ATOM	2638	CG2	VAL	A	393	25.566	21.766	17.210	1.00 13.79
MOTA	2639	N	MET	Α	394	26.592	23.298	14.312	1.00 15.41
ATOM	2640	CA	MET			27.900	23.962	14.231	1.00 16.55
ATOM	2641	C	MET	A	394	28.188	24.442	15.647	1.00 16.43
ATOM	2642	0	MET	Α	394	27.737	25.553	16.059	1.00 14.99
ATOM	2643	CB	MET	Δ	394	27.822	25.143	13.264	1.00 16.88
ATOM	2644	CG	MET			27.607	24.724	11.818	1.00 21.12
MOTA	. 2645	SD	MET			27.178	26.083	10.700	1.00 27.34
MOTA	2646	CE	MET	Α	394	25.475	25.768	10.522	1.00 26.22
ATOM	2647	N	GLY			28.909	23.622	16.406	1.00 16.28
			GLY					17.780	1.00 15.87
ATOM	2648	CA				29.220	23.967		
MOTA	2649	C	GLY			30.487	24.775	17.971	1.00 16.72
MOTA	2650	0	GLY	Α	395	31.011	25.408	17.005	1.00 16.25
MOTA	2651	N	ALA			30.989	24.769	19.202	1.00 17.29
MOTA	2652	CA	ALA			32.211	25.511	19.586	1.00 19.21
ATOM	2653	C	ALA	Α	396	33.383	25.310	18.634	1.00 19.63
ATOM	2654	0	ALA	Α	396	34.050	26.303	18.223	1.00 22.56
ATOM	2655	СВ	ALA			32.626	25.128	21.013	1.00 16.95
MOTA	2656	N	VAL			33.661	24.065	18.269	1.00 21.31
ATOM	2657	CA	VAL	A	397	34.792	23.781	17.353	1.00 23.40
ATOM	2658	С	VAL			34.690	24.592	16.068	1.00 21.89
ATOM	2659	ō				35.731	25.029	15.496	1.00 24.15
			VAL				23.029		
ATOM	2660	CB	VAL			34.874	22.274	17.012	1.00 24.19
MOTA	2661	CG1	VAL	Α	397	35.065	21.480	18.287	1.00 26.91
ATOM	2662	CG2	VAL	Α	397	33.623	21.826	16.290	1.00 25.89

ATOM	2663	N	ILE A	398	33.472	24.805	15.586	1.00 21.78
ATOM	2664		ILE A					
		CA			33.276	25.612	14.359	1.00 21.50
ATOM	2665	С	ILE A		33.403	27.086	14.735	1.00 19.91
MOTA	2666	0	ILE A	398	34.222	27.849	14.135	1.00 16.77
MOTA	2667	CB	ILE A	398	31.872	25.390	13.749	1.00 23.48
ATOM	2668	CG1	ILE A	398	31.859	24.113	12.910	1.00 26.70
ATOM	2669	CG2	ILE A		31.469	26.596	12.895	1.00 24.67
ATOM	2670	CD1	ILE A					
					32.656	24.223	11.620	1.00 27.64
MOTA	2671	N	MET A		32.614	27.492	15.726	1.00 17.64
MOTA	2672	CA	MET A		32.594	28.889	16.201	1.00 16.99
MOTA	2673	С	MET A	399	33.951	29.439	16.640	1.00 17.65
ATOM	2674	0	MET A	399	34.202	30.677	16.517	1.00 18.70
ATOM	2675	СВ	MET A	399	31.575	29.025	17.331	1.00 15.33
ATOM	2676	CG	MET A		30.138	28.800	16.866	1.00 14.30
ATOM	2677	SD	MET A		28.891	29.038		
							18.155	1.00 16.41
ATOM	2678	CE	MET A		28.972	30.826	18.388	1.00 10.15
MOTA	2679	N	GLU A		34.835	28.579	17.143	1.00 16.09
MOTA	2680	CA	GLU A	400	36.175	29.051	17.580	1.00 16.46
ATOM	2681	С	GLU A	400	36.968	29.576	16.389	1.00 14.50
MOTA	2682	0	GLU A	400	37.971	30.332	16.553	1.00 14.83
ATOM	2683	CB	GLU A	400	36.957	27.919	18.257	1.00 15.95
ATOM	2684	CG	GLU A		36.318	27.419	19.540	1.00 18.44
ATOM	2685	CD	GLU A		37.156	26.376	20.243	1.00 18.72
ATOM	2686	OE1	GLU A		37.771	25.542	19.546	1.00 20.29
MOTA	2687	OE2	GLU A		37.186	26.383	21.493	1.00 19.60
MOTA	2688	N	GLY A	401	36.544	29.204	15.190	1.00 13.62
MOTA	2689	CA	GLY A	401	37.246	29.662	14.010	1.00 15.09
ATOM	2690	С	GLY A	401	36.747	31.010	13.533	1.00 16.28
ATOM	2691	0	GLY A	401	37.435	31.693	12.716	1.00 16.14
ATOM	2692	N	PHE A		35.591	31.438	14.033	1.00 14.90
ATOM	2693	CA	PHE A		35.018	32.712	13.572	1.00 15.01
MOTA	2694	C	PHE A		34.378	33.605	14.615	1.00 15.52
ATOM	2695	0	PHE A		34.078	33.185	15.777	1.00 16.47
ATOM	2696	CB	PHE A		33.966	32.424	12.495	1.00 14.48
ATOM	2697	CG	PHE A	402	34.381	31.364	11.522	1.00 15.64
ATOM	2698	CD1	PHE A	402	34.126	30.021	11.785	1.00 14.91
MOTA	2699	CD2	PHE A	402	35.095	31.700	10.376	1.00 15.20
ATOM	2700	CE1	PHE A		34.581	29.027	10.920	1.00 15.18
ATOM	2701	CE2	PHE A		35.555	30.717	9.507	1.00 15.72
MOTA	2702	CZ	PHE A		35.298	29.376	9.782	
								1.00 15.12
ATOM	2703	N	TYR A		34.168	34.847	14.208	1.00 15.73
MOTA	2704	CA	TYR A		33.474	35.837	15.039	1.00 15.81
MOTA	2705	C	TYR A	403	32.071	35.641	14.489	1.00 14.48
ATOM	2706	0	TYR A	403	31.846	35.789	13.250	1.00 15.47
ATOM	2707	CB	TYR A	403	33.977	37.251	14.731	1.00 14.45
ATOM	2708	CG	TYR A	403	33.265	38.340	15.499	1.00 15.22
ATOM	2709		TYR A		32.899	38.152	16.834	1.00 14.85
MOTA	2710		TYR A		33.018	39.584	14.916	1.00 14.28
MOTA	2711		TYR A		32.311	39.175	17.569	1.00 15.25
MOTA	2712		TYR A		32.435	40.617	15.644	1.00 14.12
ATOM	2713	CZ	TYR A	403	32.086	40.406	16.967	1.00 15.72
MOTA	2714	OH	TYR A	403	31.525	41.427	17.697	1.00 18.09
ATOM	2715	N	VAL A	404	31.125	35.286	15.345	1.00 14.70
ATOM	2716	CA	VAL A		29.753	35.040	14.854	1.00 14.44
ATOM	2717	C	VAL A		28.759	36.079	15.342	1.00 14.92
ATOM	2718	0	VAL A				16.582	1.00 15.62
					28.552	36.259		
ATOM	2719	CB	VAL A		29.284	33.629	15.260	1.00 14.39
ATOM	2720		VAL A		27.925	33.323	14.640	1.00 11.90
MOTA	2721		VAL A		30.327	32.603	14.819	1.00 12.73
MOTA	2722	N	VAL A	405	28.136	36.762	14.386	1.00 16.06
ATOM	2723	CA	VAL A	405	27.153	37.822	14.676	1.00 14.31
ATOM	2724	С	VAL A		25.717	37.312	14.562	1.00 16.79
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ATOM	2725	0	VAL A	405	25.238	36.955	13.443	1.00 16.14
MOTA	2726	CB	VAL A	405	27.318	39.004	13.700	1.00 13.66
	2727		VAL A		26.302	40.092	14.021	1.00 12.39
MOTA								
MOTA	2728	CG2	VAL A		28.739	39.547	13.775	1.00 10.80
ATOM	2729	N	PHE A	406	25.019	37.260	15.691	1.00 16.73
ATOM	2730	CA	PHE A	406	23.616	36.805	15.685	1.00 16.71
	2731	C	PHE A		22.755	38.049	15.531	1.00 17.47
MOTA								
ATOM	2732	0	PHE A	406	22.286	38.654	16.539	1.00 17.39
ATOM	2733	CB	PHE A	406	23.287	36.053	16.979	1.00 13.96
ATOM	2734	CG	PHE A	406	24.061	34.765	17.139	1.00 13.82
		-			25.398	34.783	17.533	1.00 13.31
MOTA	2735		PHE A					
ATOM	2736		PHE A		23.464	33.538	16.863	1.00 12.85
MOTA	2737	CE1	PHE A	406	26.128	33.601	17.646	1.00 13.23
ATOM	2738	CE2	PHE A	406	24.185	32.350	16.973	1.00 12.78
ATOM	2739	CZ	PHE A		25.522	32.382	17.367	1.00 12.96
					22.566	38.449	14.278	1.00 18.08
ATOM	2740	N	ASP A					
MOTA	2741	CA	ASP A		21.785	39.647	13.932	1.00 19.70
ATOM	2742	С	ASP A	407	20.297	39.316	13.927	1.00 19.73
ATOM	2743	0	ASP A	407	19.675	39.120	12.837	1.00 18.96
ATOM	2744	CB	ASP A	407	22.221	40.153	12.552	1.00 22.61
	2745	CG	ASP A		21.663	41.530	12.223	1.00 24.28
ATOM								
MOTA	2746		ASP A		20.660	41.935	12.849	1.00 24.12
ATOM	2747	OD2	ASP A	407	22.225	42.198	11.325	1.00 23.37
MOTA	2748	N	ARG A	408	19.709	39.245	15.116	1.00 19.72
ATOM	2749	CA	ARG A	408	18.269	38.928	15.259	1.00 22.01
	2750	C	ARG A		17.393	39.967	14.557	1.00 21.56
ATOM								
ATOM	2751	0	ARG A		16.386	39.606	13.875	1.00 20.49
MOTA	2752	CB	ARG A	408	17.909	38.835	16.748	1.00 23.44
ATOM	2753	CG	ARG A	408	18.670	37.724	17.479	1.00 25.61
MOTA	2754	CD	ARG A	408	18.838	37.994	18.973	1.00 28.14
	2755	NE	ARG A		17.843	37.328	19.814	1.00 31.17
MOTA								
MOTA	2756	cz	ARG A		16.567	37.679	19.887	1.00 32.24
MOTA	2757	NH1	ARG A	408	16.127	38.693	19.163	1.00 35.70
ATOM	2758	NH2	ARG A	408	15.735	37.029	20.687	1.00 31.13
MOTA	2759	N	ALA A	409	17.750	41.241	14.694	1.00 21.10
	2760	CA	ALA A		16.978	42.329	14.056	1.00 22.43
MOTA								1.00 22.80
MOTA	2761	С	ALA A		16.785	42.050	12.571	
MOTA	2762	0	ALA A	409	15.646	42.177	12.034	1.00 24.04
ATOM	2763	CB	ALA A	409	17.689	43.664	14.247	1.00 20.85
ATOM	2764	N	ARG A	410	17.858	41.664	11.889	1.00 23.89
ATOM	2765	CA	ARG A		17.770	41.374	10.445	1.00 25.07
								1.00 24.26
MOTA	2766	C	ARG A		17.639	39.888	10.119	
MOTA	2767	0	ARG A	4 410	17.908	39.461	8.956	1.00 24.63
ATOM	2768	CB	ARG A	410	18.987	41.949	9.724	1.00 26.83
MOTA	2769	CG	ARG A	410	19.025	43.464	9.700	1.00 29.89
ATOM	2770	CD	ARG Z		19.326	43.944	8.295	1.00 32.69
						44.664		1.00 33.51
MOTA	2771	NE	ARG A		20.590		8.208	
MOTA	2772	CZ	ARG A		21.182	44.979	7.062	1.00 34.58
MOTA	2773	NH1	ARG A	410	20.626	44.631	5.907	1.00 33.99
MOTA	2774	NH2	ARG I	410	22.328	45.644	7.068	1.00 35.27
ATOM	2775	N	LYS 2		17.223	39.091	11.097	1.00 22.77
						37.630	10.891	1.00 22.97
ATOM	2776	CA	LYS A		17.061			
MOTA	2777	С	LYS I			37.031	10.104	1.00 21.80
MOTA	2778	0	LYS 2	411		36.309	9.081	1.00 20.39
MOTA	2779	CB	LYS 2	411	15.761	37.335	10.138	1.00 23.53
ATOM	2780	CG	LYS			37.686	10.886	1.00 27.80
	2781	CD	LYS 2			37.188	10.121	1.00 30.25
ATOM								1.00 31.18
MOTA	2782	CE	LYS			35.678	9.890	
MOTA	2783	NZ	LYS 2			35.163	9.142	1.00 34.08
ATOM	2784	N	ARG 2	412	19.449	37.290	10.541	1.00 19.85
MOTA	2785	CA	ARG 2	412	20.607	36.748	9.815	1.00 18.29
ATOM	2786	C	ARG Z			36.505	10.736	1.00 18.54
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MOTA	2787	0	ARG A	412	21.911	37.137	11.837	1.00 18.56
ATOM	2788	CB	ARG A	412	21.019	37.714	8.703	1.00 18.72
	2789.	CG	ARG A		21.571	39.027	9.239	1.00 18.66
MOTA								
ATOM	2790	CD	ARG A		21.941	39.988	8.127	1.00 18.34
ATOM	2791	NE	ARG A	412	22.560	41.196	8.662	1.00 19.28
MOTA	2792	CZ	ARG A	412	23.082	42.163	7.916	1.00 20.03
	2793	NH1			23.059	42.067	6.591	1.00 19.36
ATOM								
MOTA	2794	NH2	ARG A		23.635	43.219	8.496	1.00 19.27
MOTA	2795	N	ILE A	413	22.668	35.606	10.317	1.00 17.01
ATOM	2796	CA	ILE A	413	23.865	35.285	11.103	1.00 16.43
MOTA	2797	C	ILE A		25.103	35.576	10.266	1.00 16.20
ATOM	2798	0	ILE A		25.213	35.125	9.084	1.00 17.17
MOTA	2799	CB	ILE A	413	23.855	33.808	11.533	1.00 16.02
ATOM	2800	CG1	ILE A	413	22.667	33.562	12.469	1.00 13.92
ATOM	2801	CG2	ILE A	413	25.168	33.458	12.218	1.00 15.95
ATOM	2802	CD1	ILE A		22.482	32.130	12.862	1.00 14.89
MOTA	2803	N	GLY A		26.028	36.332	10.841	1.00 15.43
MOTA	2804	CA	GLY A	414	27.243	36.679	10.132	1.00 14.42
MOTA	2805	С	GLY A	414	28.463	35.899	10.585	1.00 14.91
ATOM	2806	0	GLY A	414	28.569	35.463	11.779	1.00 12.74
			PHE A		29.392	35.709	9.656	1.00 12.70
ATOM	2807	N						
ATOM	2808	CA	PHE A		30.638	34.977	9.932	1.00 14.84
MOTA	2809	С	PHE A	415	31.823	35.766	9.403	1.00 15.05
ATOM	2810	0	PHE A	415	31.761	36.376	8.291	1.00 17.34
ATOM	2811	CB	PHE A		30.613	33.599	9.256	1.00 13.57
	2812	CG	PHE A		29.628	32.640	9.860	1.00 13.35
MOTA								
MOTA	2813	CD1			30.034	31.710	10.820	1.00 14.56
MOTA	2814	CD2	PHE A	415	28.296	32.660	9.472	1.00 11.54
ATOM	2815	CE1	PHE A	415	29.117	30.809	11.383	1.00 13.74
MOTA	2816	CE2	PHE A	415	27.373	31.768	10.027	1.00 12.67
					27.787	30.839	10.985	1.00 13.15
MOTA	2817	CZ	PHE A					
ATOM	2818	N	ALA A		32.895	35.779	10.178	1.00 15.11
ATOM	2819	CA	ALA A	416	34.135	36.470	9.786	1.00 14.57
MOTA	2820	С	ALA A	416	35.248	35.738	10.515	1.00 14.48
ATOM	2821	ō	ALA A		35.027	35.186	11.639	1.00 12.56
								1.00 11.46
ATOM	2822	CB	ALA A		34.095	37.935	10.208	
MOTA	2823	N	VAL A	417	36.425	35.692	9.906	1.00 14.71
ATOM	2824	CA	VAL A	417	37.569	35.011	10.528	1.00 16.80
ATOM	2825	С	VAL A	417	37.835	35.634	11.892	1.00 18.08
ATOM	2826	ō	VAL A		37.922	36.901	12.033	1.00 17.13
						35.126	9.642	1.00 17.67
ATOM	2827	СВ	VAL A		38.824			
ATOM	2828		VAL A		40.022	34.486	10.333	1.00 16.83
ATOM	2829	CG2	VAL A	417	38.561	34.441	8.301	1.00 18.32
ATOM	2830	N	SER A	418	37.953	34.785	12.905	1.00 17.31
ATOM	2831	CA	SER A		38.201	35.271	14.272	1.00 17.62
						35.712	14.455	1.00 18.36
ATOM	2832	C	SER A		39.637			
MOTA	2833	0	SER A	418	40.591	35.038	13.963	1.00 19.44
ATOM	2834	CB	SER A	418	37.882	34.182	15.295	1.00 18.09
ATOM	2835	OG	SER A	418	38.228	34.617	16.599	1.00 17.42
ATOM	2836	N	ALA A		39.821	36.827	15.150	1.00 17.60
								1.00 18.46
ATOM	2837	CA	ALA A		41.175	37.335	15.410	
ATOM	2838	С	ALA A	419	41.877	36.423	16.423	1.00 19.09
ATOM	2839	Ö	ALA A	419	43.117	36.553	16.649	1.00 19.60
ATOM	2840	СВ	ALA A		41.106	38.772	15.943	1.00 17.70
MOTA	2841	N	CYS A		41.132	35.500	17.032	1.00 19.36
								1.00 20.89
ATOM	2842	CA	CYS A		41.736	34.575	18.029	
MOTA	2843	С	CYS A	420	41.677	33.105	17.624	1.00 19.60
ATOM	2844	0	CYS A		41.805	32.202	18.501	1.00 22.74
ATOM	2845	CB	CYS A		41.064	34.734	19.410	1.00 21.69
					39.353	34.096	19.526	1.00 25.02
ATOM	2846	SG	CYS A					
ATOM	2847	N	HIS A		41.495	32.814	16.342	1.00 17.86
MOTA	2848	CA	HIS A	421	41.435	31.393	15.933	1.00 17.71
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MOTA	2849	С	HIS A	421	42.834	30.798	15.799	1.00 17.18
ATOM	2850	0	HIS A	421	43.801	31.495	15.356	1.00 14.17
ATOM	2851	CB	HIS A		40.641	31.236	14.625	1.00 18.65
MOTA	2852	CG	HIS A	421	41.433	31.504	13.381	1.00 18.77
	2853		HIS A		42.114	30.514	12.705	1.00 18.84
ATOM								
ATOM	2854	CD2	HIS A	421	41.631	32.645	12.678	1.00 18.73
MOTA	2855	CE1	HIS A	421	42.695	31.032	11.637	1.00 17.98
ATOM	2856	NE2	HIS A	421	42.418	32.323	11.597	1.00 20.03
ATOM	2857	N	VAL A	422	42.965	29.533	16.194	1.00 16.96
MOTA	2858	CA	VAL A		44.260	28.816	16.132	1.00 16.89
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ATOM	2859	С	VAL A	422	44.571	28.334	14.719	1.00 17.53
ATOM	2860	0	VAL A	422	43.678	27.764	14.021	1.00 17.13
MOTA	2861	CB	VAL A		44.257	27.588	17.061	1.00 16.92
ATOM	2862	CG1	VAL A	422	45.632	26.938	17.063	1.00 15.15
ATOM	2863	CG2	VAL A	422	43.850	28.004	18.479	1.00 19.33
ATOM	2864	N	HIS A	423	45.815	28.531	14.291	1.00 16.64
ATOM	2865	CA	HIS A	423	46.264	28.112	12.940	1.00 16.92
	2866	С	HIS A		47.792	28.038	12.906	1.00 17.46
MOTA								
MOTA	2867	0	HIS A	423	48.461	28.105	13.981	1.00 17.20
ATOM	2868	CB	HIS A	423	45.755	29.111	11.889	1.00 15.85
					46.242	30.512	12.096	1.00 18.62
MOTA	2869	CG	HIS A					
ATOM	2870	ND1	HIS A	423	47.390	30.998	11.504	1.00 19.80
ATOM	2871	CD2	HIS A	423	45.758	31.522	12.857	1.00 17.42
MOTA	2872		HIS A		47.590	32.245	11.892	1.00 18.22
ATOM	2873	NE2	HIS A	423	46.615	32.586	12.714	1.00 18.53
ATOM	2874	N	ASP A		48.360	27.869	11.714	1.00 18.00
MOTA	2875	CA	ASP A	424	49.836	27.817	11.556	1.00 17.75
MOTA	2876	С	ASP A	424	50.194	28.804	10.453	1.00 18.36
	2877	Ö	ASP A		49.294	29.527	9.935	1.00 20.02
MOTA								
ATOM	2878	СB	ASP A	424	50.305	26.396	11.206	1.00 18.00
MOTA	2879	CG	ASP A	424	49.545	25.791	10.037	1.00 19.08
						24.623	10.149	1.00 18.99
MOTA	2880	OD1			49.110			
ATOM	2881	OD2	ASP A	424	49.390	26.473	9.003	1.00 20.46
ATOM	2882	N	GLU A	425	51.459	28.877	10.063	1.00 17.55
							9.015	1.00 18.77
MOTA	2883	CA	GLU A		51.813	29.853		
ATOM	2884	C	GLU A	425	51.497	29.379	7.601	1.00 16.95
ATOM	2885	0	GLU A	125	51.724	30.131	6.613	1.00 17.24
MOTA	2886	CB	GLU A	425	53.289	30.239	9.112	1.00 18.65
ATOM	2887	CG	GLU A	425	54.254	29.150	8.714	1.00 20.84
ATOM	2888	CD	GLU A		55.632	29.697	8.381	1.00 21.89
MOTA	2889	OE1	GLU A	425	56.481	28.901	7.936	1.00 22.61
ATOM	2890	OE2	GLU A	425	55.867	30.920	8.559	1.00 22.65
	2891		PHE A		50.955	28.171	7.476	1.00 14.60
MOTA	_	N						
MOTA	2892	CA	PHE A	426	50.619	27.606	6.150	1.00 13.51
MOTA	2893	С	PHE A	426	49.157	27.767	5.763	1.00 15.14
					48.826	27.822	4.540	1.00 16.10
MOTA	2894	0	PHE A					
MOTA	2895	CB	PHE A	426	51.001	26.127	6.109	1.00 14.53
ATOM	2896	CG	PHE A	426	52.452	25.877	6.400	1.00 14.20
							5.482	1.00 13.59
MOTA	2897		PHE A		53.433	26.244		
MOTA	2898	CD2	PHE A	426	52.841	25.298	7.606	1.00 14.11
ATOM	2899		PHE A		54.787	26.040	5.762	1.00 14.83
								1.00 15.49
MOTA	290.0	CE2	PHE A		54.192	25.087	7.897	
MOTA	2901	CZ	PHE A	426	55.167	25.460	6.969	1.00 14.08
	2902	N	ARG A		48.269	27.827	6.752	1.00 13.77
ATOM								
ATOM	2903	CA	ARG A	427	46.824	27.985	6.469	1.00 14.89
MOTA	2904	С	ARG A	427	46.130	28.695	7.615	1.00 15.43
	2905	Õ	ARG A		46.630	28.710	8.781	1.00 14.58
ATOM								
MOTA	2906	CB	ARG A	427	46.132	26.632	6.301	1.00 15.33
MOTA	2907	CG	ARG A	427	46.959	25.518	5.707	1.00 16.84
	2908		ARG A		46.645	24.234	6.477	1.00 17.68
ATOM		CD						
MOTA	2909	NE	ARG A	427	45.994	23.230	5.655	1.00 16.69
MOTA	2910	CZ	ARG A	427	45.701	21.998	6.062	1.00 15.45

MOTA	2911	NH1	ARG A	427	45.114	21.159	5.224	1.00 14.20
ATOM	2912	NH2	ARG A	427	45.981	21.603	7.296	1.00 13.31
			THR A		44.976	29.269	7.317	1.00 15.28
MOTA	2913	N						
ATOM	2914	CA	THR A	428	44.180	29.967	8.336	1.00 17.94
ATOM	2915	C	THR A	428	42.731	29.650	8.041	1.00 16.25
ATOM	2916	0	THR A	428	42.400	29.165	6.923	1.00 14.77
			THR A		44.353	31.503	8.249	1.00 18.18
ATOM	2917	СВ						
ATOM	2918	OG1	THR A	428	44.043	31.942	6.921	1.00 20.24
ATOM	2919	CG2	THR A	428	45.773	31.901	8.583	1.00 19.84
ATOM	2920	N	ALA A	429	41.860	29.901	9.009	1.00 16.14
ATOM	2921	CA	ALA A		40.423	29.677	8.803	1.00 16.03
					*			
ATOM	2922	С	ALA A		40.048	30.739	7.775	1.00 15.66
ATOM	2923	0	ALA A	429	40.808	31.738	7.574	1.00 14.51
ATOM	2924	CB	ALA A	429	39.656	29.898	10.105	1.00 17.08
ATOM	2925	N	ALA A	430	38.920	30.575	7.107	1.00 14.04
			ALA A		38.556	31.576	6.100	1.00 13.71
ATOM	2926	CA						
ATOM	2927	С	ALA A		37.067	31.706	5.883	1.00 11.98
ATOM	2928	0	ALA A	430	36.271	30.754	6.166	1.00 12.33
ATOM	2929	CB	ALA A	430	39.251	31.246	4.762	1.00 12.27
ATOM	2930	N	VAL A	431	36.671	32.874	5.396	1.00 11.01
			VAL A		35.260	33.149	5.076	1.00 13.39
MOTA	2931	CA						
ATOM	2932	С	VAL A		35.344	33.773	3.697	1.00 15.69
MOTA	2933	0	VAL A	431	35.857	34.926	3.533	1.00 17.86
ATOM	2934	CB	VAL A	431	34.624	34.145	6.056	1.00 11.50
ATOM	2935		VAL A		33.148	34.294	5.737	1.00 10.61
					34.818	33.659	7.494	1.00 10.71
MOTA	2936		VAL A					
MOTA	2937	. N	GLU A		34.874	33.048	2.694	1.00 16.74
MOTA	2938	CA	GLU A	432	34.969	33.544	1.320	1.00 18.65
ATOM	2939	С	GLU A	432	33.681	33.414	0.530	1.00 18.40
ATOM	2940	ō	GLU A		32.794	32.567	0.852	1.00 16.81
	•					32.796	0.607	1.00 19.91
ATOM	2941	СВ	GLU A		36.097			
ATOM	2942	CG	GLU A		37.460	33.031	1.241	1.00 24.66
ATOM	2943	CD	GLU A	432	38.466	31.930	0.935	1.00 27.80
ATOM	2944	OE1	GLU A	432	39.681	32.196	1.051	1.00 30.84
ATOM	2945	OE2	GLU A		38.049	30.799	0.595	1.00 28.87
					33.574	34.243	-0.504	1.00 18.95
ATOM	2946	N	GLY A					
MOTA	2947	CA	GLY A	433	32.408	34.244	-1.363	1.00 19.36
ATOM	2948	C	GLY A	433	32.504	35.385	-2.359	1.00 19.59
ATOM	2949	0	GLY A	433	33.489	36.173	-2.328	1.00 18.33
MOTA	2950	N	PRO A		31.511	35.539	~3.243	1.00 19.47
			PRO A		30.345	34.655	-3.285	1.00 19.72
ATOM	2951	CA						
MOTA	2952	С	PRO A		30.485	33.589	-4.353	1.00 19.98
ATOM	2953	0	PRO A	434	31.382	33.674	-5.235	1.00 22.24
MOTA	2954	CB	PRO A	434	29.215	35.619	-3.595	1.00 19.80
ATOM	2955	CG	PRO A	434	29.869	36.517	-4.616	1.00 19.70
	2956	CD	PRO A		31.261	36.770	-4.018	1.00 19.73
ATOM								
ATOM	2957	И	PHE A		29.624	32.583	-4.290	1.00 21.45
MOTA	2958	CA	PHE A	435	29.619	31.502	-5.292	1.00 22.31
ATOM	2959	С	PHE A	435	28.217	31.513	-5.872	1.00 24.39
ATOM	2960	0	PHE A		27.207	31.636	-5.110	1.00 24.58
					29.924	30.155	-4.636	1.00 22.02
ATOM	2961	СВ	PHE A					
ATOM	2962	CG	PHE A		31.215	30.141	-3.876	1.00 20.80
MOTA	2963	CD1	PHE A	435	31.232	30.392	-2.507	1.00 20.70
ATOM	2964		PHE A		32.424	29.945	-4.542	1.00 21.70
ATOM	2965		PHE A		32.432	30.451	-1.809	1.00 20.27
					33.634	30.003	-3.853	1.00 21.68
MOTA	2966		PHE A					
ATOM	2967	CZ	PHE A		33.637	30.259	-2.481	1.00 21.51
MOTA	2968	N	VAL A	436	28.117	31.396	-7.192	1.00 27.02
ATOM	2969	CA	VAL A	436	26.802	31.438	-7.872	1.00 29.79
MOTA	2970	C	VAL A		26.526	30.219	-8.739	1.00 32.85
ATOM	2971	o	VAL A		25.434	30.120	-9.376	1.00 33.81
								1.00 28.98
MOTA	2972	CB	VAL A	436	26.702	32.677	-8.787	1.00 20.90

MOTA	2973	CG1	VAL A	436	26.999	33.944	-7.996	1.00 29.00
MOTA	2974	CG2	VAL A		27.678	32.537	-9.947	1.00 28.49
MOTA	2975	N	THR A	437	27.473	29.292	-8.795	1.00 36.05
MOTA	2976	CA	THR A		27.305	28.089	-9.638	1.00 39.30
MOTA	2977	С	THR A	437	26.582	26.979	-8.870	1.00 41.99
ATOM	2978	0	THR A		26.604	25.775	-9.276	1.00 41.77
MOTA	2979	CB	THR A	437	28.690		-10.123	1.00 39.02
MOTA	2980	OG1	THR A	437	28.552	26.981	-11.408	1.00 42.51
MOTA	2981	CG2	THR A	437	29.280	26.578	-9.156	1.00 38.10
ATOM	2982	N	LEU A	438	25.908	27.368	-7.794	1.00 45.33
ATOM	2983	CA	LEU A	438	25.199	26.417	-6.901	1.00 49.22
MOTA	2984	С	LEU A	438	23.753	26.016	-7.165	1.00 50.49
MOTA	2985	0	LEU A	438	22.869	26.878	-7.466	1.00 51.99
ATOM	2986	CB	LEU A	438	25.276	26.944	-5.473	1.00 50.30
MOTA	2987	CG	LEU A	438	26.027	28.269	-5.358	1.00 50.73
MOTA	2988	CD1	LEU A	438	25.108	29.457	-5.584	1.00 50.27
ATOM	2989	CD2	LEU A		26.629	28.328	-4.001	1.00 51.67
MOTA	2990	N	ASP A		23.505	24.715	-7.037	1.00 52.67
ATOM	2991	CA	ASP A	439	22.149	24.128	-7.172	1.00 55.74
MOTA	2992	С	ASP A	439	21.690	24.224	-5.722	1.00 56.96
MOTA	2993	0	ASP A		21.757	23.221	-4.945	1.00 57.33
MOTA	2994	СВ	ASP A	439	22.240	22.657	-7.586	1.00 56.39
MOTA	2995	CG	ASP A	439	20.879	21.993	-7.695	1.00 57.68
MOTA	2996	OD1	ASP A	439	20.046	22.178	-6.781	1.00 57.75
ATOM	2997	OD2	ASP A	439	20.645	21.274	-8.692	1.00 58.18
MOTA	2998	N	MET A	440	21.233	25.407	-5.337	1.00 58.71
MOTA	2999	CA	MET A		20.841	25.656	-3.944	1.00 60.87
MOTA	3000	С	MET A	440	19.435	26.215	-3.713	1.00 62.52
MOTA	3001	0	MET A	440	19.247	27.451	-3.489	1.00 63.93
MOTA	3002	CB	MET A		21.916	26.569	-3.346	1.00 60.48
ATOM	3003	CG	MET A	440	21.523	27.456	-2.201	1.00 60.72
MOTA	3004	SD	MET A	440	22.755	28.755	-2.086	1.00 59.28
MOTA	3005	CE	MET A		22.367	29.689	-3.543	1.00 59.46
MOTA	3006	N	GLU A		18.435	25.343	•	1.00 63.61
MOTA	3007	CA	GLU A	441	17.042	25.774	-3.514	1.00 65.54
ATOM	3008	С	GLU A		16.356	24.847	-2.518	1.00 64.49
MOTA	3009	0	GLU A		15.998	25.285	-1.375	1.00 65.36
MOTA	3010	CB	GLU A		16.229	25.847	-4.815	1.00 67.99
MOTA	3011	CG	GLU A		16.500	24.745	-5.822	1.00 70.98
MOTA	3012	CD	GLU A		17.353	25.228	-6.981	1.00 72.23
ATOM	3013		GLU A		18.507	25.646	-6.742	1.00 73.24 1.00 73.30
MOTA	3014	OE2			16.867	25.194		1.00 73.30 1.00 61.29
MOTA	3015	N	ASP A		16.170	23.585	-2.896	1.00 51.29
MOTA	3016	CA			15.519	22.616		1.00 55.47
MOTA	3017	G.	ASP A		16.504	21.966		1.00 54.59
MOTA	3018	0	ASP A		16.615	20.704 21.530		1.00 59.93
MOTA	3019	CB	ASP A		14.800			1.00 60.90
MOTA	3020	CG	ASP A		13.298	21.616		1.00 61.34
MOTA	3021		ASP A		12.689 12.729	22.478		1.00 61.81
MOTA	3022		ASP A			20.832		1.00 51.31
MOTA	3023	N	CYS A		17.207	22.790		1.00 47.79
MOTA	3024	CA	CYS A		18.200	22.281 22.156		1.00 46.40
ATOM	3025	C	CYS A		17.635		2.121	1.00 44.04
MOTA	3026	0	CYS A		18.168 19.421	21.373 23.198		1.00 48.61
MOTA	3027	CB	CYS A		20.176			1.00 46.95
MOTA	3028	SG	CYS A		16.566	23.339 22.895		1.00 45.40
ATOM	3029	N	GLY A		15.953	22.895		1.00 45.06
ATOM	3030	CA	GLY A		15.933	22.846		1.00 45.25
ATOM	3031	C	GLY A		14.271	21.6/3		1.00 44.97
MOTA	3032	0	GLY A		15.018	21.204	•	1.00 44.97
ATOM	3033	N	TYR A		14.140	19.968		1.00 44.48
MOTA	3034	CA	TYR A	445	14.140	12.708	J.441	1.00 11.10

MOTA	3035	С	TYR	Α	445	12.778	20.467	5.882	1.00 45.23
ATOM	3036	0	TYR			12.662	21.558	6.530	1.00 44.57
									-
ATOM	3037	CB	TYR			14.801		6.531	1.00 43.11
ATOM	3038	CG	TYR	Α	445	13.918	17.997	6.871	1.00 42.75
ATOM	3039	CD1	TYR	Α	445	13.846	16.905	6.010	1.00 42.58
ATOM	3040	CD2				13.170		8.049	1.00 42.27
MOTA	3041		TYR			13.042		6.327	1.00 41.99
ATOM	3042	CE2	TYR	Α	445	12.358	16.917	8.360	1.00 43.20
ATOM	3043	CZ	TYR	А	445	12.289	15.835	7.503	1.00 41.98
ATOM	3044	OH	TYR			11.490		7.810	1.00 20.00
ATOM	3045	N	ASN			11.746		5.550	1.00 45.69
MOTA	3046	CA	ASN	Α	446	10.359	20.012	5.947	1.00 48.64
ATOM.	3047.	С	ASN	Α	446	9.776	18.726	6.524	1.00 50.90
ATOM	3048	0	ASN	Α	446	9.894	17.625	5.896	1.00 51.59
	3049	СВ	ASN			9.537		4.738	1.00 48.19
ATOM									
ATOM	3050	CG	ASN			9.975		4.213	1.00 48.18
ATOM	3051	OD1	ASN	A	446	9.926	22.858	4.950	1.00 48.63
ATOM	3052	ND2	ASN	Α	446	10.403	21.867	2.957	1.00 48.04
ATOM	3053	N	ILE	А	447	9.165	18.826	7.700	1.00 53.94
ATOM	3054	CA	ILE			8.569		8.388	1.00 55.99
MOTA	3055	С	ILE			7.720		7.463	1.00 57.01
ATOM	3056	0	ILE	A	447	7.449	17.195	6.318	1.00 58.11
MOTA	3057	CB	ILE	Α	447	7.699	18.105	9.577	1.00 55.86
ATOM	3058		ILE	Α	447	8.488	19.086	10.450	1.00 56.28
	3059	CG2	ILE			7.267		10.406	1.00 56.92
MOTA									
MOTA	3060	CD1				9.759		11.037	1.00 55.79
MOTA	3061	oxt	ILE	Α	447	7.328	15.666	7.895	1.00 57.55
ATOM	3062	N	SER	Ρ	1	35.528	15.672	28.238	1.00 37.61
ATOM	3063	CA	SER	P	1	34.172	16.082	28.590	1.00 36.72
	3064	C	SER		1	33.508		27.450	1.00 34.75
MOTA									
MOTA	3065	0	SER		1	34.132		26.742	1.00 36.46
MOTA	3066	CB	SER	P	1	34.248	16.949	29.848	1.00 37.77
MOTA	3067	OG	SER	P	1	33.152	17.865	29.853	1.00 40.82
ATOM	3068	N	GLU		2	32.203		27.257	1.00 32.86
							_	26.129	1.00 32.80
ATOM	3069	CA	GLU		2	31.513			
MOTA	3070	С	GLU		2	30.218		26.552	1.00 31.23
MOTA	3071	0	GLU	₽	2	29.435	17.401	27.348	1.00 31.31
MOTA	3072	СВ	GLU	Р	2	31.275	. 16.167	25.027	1.00 33.64
ATOM	3073	CG	GLU		2	31.096		23.826	1.00 37.41
		CD	GLU			31.076		22.852	1.00 38.37
ATOM	3074				2				
MOTA	3075		GLU		2	31.996		22.983	1.00 39.04
MOTA	3076	OE2	GLU	P	2	30.175		22.037	1.00 39.43
ATOM	3077	N	VAL	₽	3	29.742	19.344	26.106	1.00 27.98
MOTA	3078	CA	VAL	P	3	28.367	19.820	26.101	1.00 26.44
	3079	C	VAL		3	27.717		24.735	1.00 26.26
MOTA									
MOTA	3080	0	VAL		3	28.371		23.701	1.00 25.48
MOTA	3081	CB	VAL	P	3	28.377		26.429	1.00 25.89
ATOM	3082	CG1	VAL	P	3	28.684	21.516	27.911	1.00 27.07
ATOM	3083		VAL		3	29.431	22.012	25.594	1.00 23.97
ATOM	3084	N	ASN		4	26.361		25.174	1.00 25.89
									1.00 26.64
MOTA	3085	CA	ASN		4	25.421		24.075	
MOTA	3086	C	ASN	P	. 4	24.027		24.452	1.00 26.87
MOTA	3087	0	ASN	P	4	23.116	19.163	25.077	1.00 27.10
MOTA	3088	СВ	ASN	P	4	25.349	17.766	23.876	1.00 27.95
ATOM	3089	CG	ASN		4	26.498		22.971	1.00 29.39
									1.00 31.90
MOTA	3090		ASN		4	26.499		21.723	
MOTA	3091	ND2	ASN		4	27.489		23.603	1.00 31.97
MOTA	3092	N	STA	Ρ	5	24.115	21.101	24.323	1.00 25.26
MOTA	3093	CA	STA		5	22.965	21.865	24.929	1.00 25,83
ATOM	3094	СВ	STA		5	23.683		26.021	1.00 27.28
					5	24.378		27.197	1.00 28.07
MOTA	3095	CG	STA						
MOTA	3096	CD1	STA	P	5	25.002	23.077	28.182	1.00 27.46

ATOM	3097	CD2	STA	Р	5		23.280	21.130	27.828	1.00 25.4	17
			STA		5		22.223	22.851	23.940	1.00 25.8	36
ATOM	3098	СН									
ATOM	3099	OH	STA	P	5		23.028	23.679	23.298	1.00 25.2	
MOTA	3100	CM	STA	₽	5		21.372	21.980	23.048	1.00 27.3	Ll
ATOM	3101	С	STA	P	5		20.420	21.340	24.125	1.00 27.8	31
			STA		5		20.241	20.065	24.095	1.00 25.7	
ATOM	3102	0									
MOTA	3103	N	VAL		6		19.339	22.479	23.764	1.00 26.0	
MOTA	3104	CA	VAL	₽	6		18.037	21.953	24.156	1.00 27.1	12
ATOM	3105	С	VAL	P	6		17.496	20.965	23.121	1.00 27.3	36
	3106	Ö	VAL		6		17.795	21.029	21.936	1.00 26.9	
ATOM											
MOTA	3107	СВ	VAL		6		17.073	23.130	24.312	1.00 27.1	
ATOM	3108	CG1	VAL	P	6		16.433	23.463	22.965	1.00 26.7	70
ATOM	3109	CG2	VAL	P	6		15.985	22.781	25.311	1.00 28.7	74
ATOM	3110	N	ALA		7		16.702	19.998	23.617	1.00 28.6	58
							16.158	18.986	22.720	1.00 32.3	
ATOM	3111	CA	ALA		7						
MOTA	3112	С	ALA		7		14.774	19.377	22.197	1.00 32.9	
ATOM	3113	0	ALA	P	7		14.040	20.149	22.801	1.00 32.0	38
ATOM	3114	СВ	ALA	P	7		16.072	17.666	23.489	1.00 31.3	38
ATOM	3115	N	GLU		8		14.443	18.843	21.007	1.00 36.3	1.0
									20.418	1.00 39.9	
MOTA	3116	CA	GLU		8		13.144	19.143			
ATOM	3117	С	GLU	P	8		12.012	18.425	21.158	1.00 41.	
ATOM	3118	0	GLU	P	8		12.189	17.359	21.733	1.00 41.	52
ATOM	3119	СВ	GLU		8		13.172	18.705	18.952	1.00 39.8	88
		CG	GLU		8		14.037	19.626	18.090	1.00 41.0	
MOTA	3120									1.00 41.0	
MOTA	3121	CD	GLU		8		13.896	19.235	16.637		
ATOM	3122	OE1	GLÜ	P	8		14.911	19.052	15.979	1.00 41.0	60
ATOM	3123	OE2	GLU	Ρ	8		12.765	19.124	16.169	1.00 41.	88
ATOM	3124	N	PHE	P	9		10.811	18.986	21.162	1.00 45.0	62
			PHE		9		9.677	18.356	21.865	1.00 49.	
MOTA	3125	CA									
ATOM	3126	С	PHE		9		9.382	16.960	21.337	1.00 50.	
ATOM	3127	0	PHE	Ρ	9		9.156	16.839	20.116	1.00 51.3	
ATOM	3128	CB	PHE	P	9		8.451	19.245	21.670	1.00 50.	65
ATOM	3129	CG	PHE		9		8.607	20.501	22.499	1.00 52.4	48
							8.278	20.493	23.849	1.00 52.	
MOTA	3130		PHE		9						
MOTA	3131	CD2	PHE	P	9		9.073	21.659	21.899	1.00 53.	
MOTA	3132	CE1	PHE	P	9		8.420	21.651	24.600	1.00 53.	74
MOTA	3133	CE2	PHE	P	9		9.215	22.817	22.659	1.00 53.	61
ATOM	3134	CZ	PHE		9		8.890	22.817	24.010	1.00 54.3	24
							9.383	16.011	22.152	1.00 51.	
ATOM	31:35	OXT	PHE		9						
MOTA	3136	OH2	TIP		2		37.673	4.149	14.933	1.00 18.	
MOTA	3137	OH2	TIP	C	3		37.999	19.019	28.545	1.00 20.	
ATOM	3138	OH2	TIP	С	12		46.550	23.555	9.446	1.00 16.	05
MOTA	3139	OH2	TIP	C	14		18.354	26.505	28.719	1.00 14.	14
			TIP		15		33.073	10.884	15.835	1.00 14.	
MOTA	3140									1.00 11.	
ATOM	3141		TIP		16		15.032	34.698	31.070		
MOTA	3142	OH2	TIP	С	17		7.170	35.908	33.277	1.00 16.	
MOTA	3143	OH2	TIP	С	19		16.624	32.704	28.166	1.00 15.	
ATOM	3144		TIP		20		35.078	42.552	29.609	1.00 19.	72
	3145				21		40.457	30.360	27.755	1.00 16.	
MOTA		OH2	TIP			•				1.00 20.	
MOTA	3146	OH2	TIP		22		52.263	20.430	9.725		
MOTA	3147	OH2	TIP	С	23		20.720	20.412	14.822	1.00 12.	
MOTA	3148	OH2	TIP	С	24		33.413	15.317	~5.393	1.00 15.	90
ATOM	3149	OH2	TIP		25		38.275	25.072	23.469	1.00 13.	40
							16.591	21.729	7.186	1.00 19.	
MOTA	3150	OH2			27						
MOTA	3151	OH2			28		21.798	19.346	19.780	1.00 14.	
MOTA	3152	OH2	TIP	С	29		17.533	34.724	25.177	1.00 16.	
MOTA	3153		TIP		30		29.162	27.768	25.821	1.00 19.	
MOTA	3154	OH2			31		40.631	28.021	16.946	1.00 14.	
							32.428	32.415	17.998	1.00 10.	
ATOM	3155	OH2	TIP		32					1.00 23.	
MOTA	3156		TIP		33		11.884	34.798	21.161	1.00 23.	10
MOTA	3157	OH2	TIP	С	34		27.837	25.769	-5.173	1.00 33.	
MOTA	3158		TIP		35		12.372	31.279	28.339	1.00 16.	96
				_				•			

MOTA	3159	он2	TIP C	36		39.263	28.648	25.755	1.00	9.84
ATOM	3160	OH2	TIP C	40		38.924	30.840	30.171	1.00	13.35
ATOM	3161	OH2	TIP C	41		18.085	18.989	18.858		16.60
	3162	OH2	TIP C	42		7.300	35.692	30.168		19.22
MOTA										
ATOM	3163	OH2	TIP C	43		14.250	32.017	30.405		18.32
MOTA	3164	он2	TIP C	44		37.440	22.761	1.333		23.96
MOTA	3165	OH2	TIP C	45		29.932	39.949	32.969		22.64
MOTA	3166	OH2	TIP C	46		29.433	17.902	20.935	1.00	16.15
MOTA	3167	OH2	TIP C	47		53.536	22.468	21.774	1.00	21.62
ATOM	3168	OH2	TIP C	48		40.180	15.699	-0.272	1.00	12.15
ATOM	3169	он2	TIP C	49		14.955	25.973	25.745	1.00	11.98
ATOM	3170	OH2	TIP C	50		38.595	6.527	3.885		23.66
		OH2	TIP C	51		48.551	24.793	17.574		18.30
ATOM	3171						27.407	17.869	1.00	8.25
MOTA	3172	OH2	TIP C	52		20.747				
MOTA	3173	OH2	TIP C	53		26.489	18.730	30.746		26.59
MOTA	3174	OH2	TIP C	54		38.723	11.162	19.249		11.49
ATOM	3175	OH2	TIP C	55		33.881	26.191	31.382		19.21
MOTA	3176	OH2	TIP C	56		13.322	31.213	40.027	1.00	15.61
MOTA	3177	OH2	TIP C	57		19.497	16.134	41.439		26.82
ATOM	3178	он2	TIP C	58		38.469	37.062	5.695	1.00	23.10
ATOM	3179	OH2	TIP C	59		45.575	15.894	3.122	1.00	18.45
MOTA	3180	OH2	TIP C	60		39.615	25.333	-1.743	1.00	20.09
ATOM	3181	OH2	TIP C	61		32.158	37.928	32.431		12.17
		OH2	TIP C	62		46.793	19.609	22.823		19.81
MOTA	3182						37.031	-0.659		29.98
MOTA	3183	OH2	TIP C	63		24.847				
MOTA	3184	OH2	TIP C	64		45.957	18.715	3.836		18.88
MOTA	3185	OH2	TIP C	65		36.189	33.100	17.653		10.63
MOTA	3186	OH2	TIP C	66		31.177	25.020	24.150		28.40
MOTA	3187	OH2	TIP C	67		46.181	23.210	18.466		20.41
MOTA	3188	OH2	TIP C	68		21.756	10.923	7.943	1.00	22.80
MOTA	3189	OH2	TIP C	69		12.936	36.695	30.481	1.00	17.63
ATOM	3190	OH2	TIP C	70		33.713	44.843	8.382	1.00	30.49
ATOM	3191	OH2	TIP C	71		21.051	41.550	39.982	1.00	31.15
MOTA	3192	OH2	TIP C	72		26.815	38.732	3.198	1.00	22.61
MOTA	3193		TIP C	73		41.656	24.820	21.177	1.00	19.69
ATOM	3194	OH2		74		25.521	30.139	47.617	1.00	31.08
ATOM	3195	OH2	TIP C	75		20.497	46.537	15.336	1.00	29.67
ATOM	3196	OH2	TIP C	76	•	7.708	28.422	41.027	1.00	26.00
ATOM	3197	OH2		77		25.650	18.585	27.821		17.30
ATOM	3198	OH2		78		35.124	16.582	21.374		15.44
		OH2		79		16.806	29.258	45.952		22.64
ATOM	3199	OH2		80		29.365	7.305	14.767		28.00
MOTA	3200					36.259	9.577	-0.018		36.72
MOTA	3201	OH2		81				35.367		29.64
ATOM	3202	OH2		82		5.598	37.375 22.267	9.863		20.30
ATOM	3203		TIP C	83		14.256				35.70
ATOM	3204		TIP C	84		34.533	14.826	41.318		22.15
MOTA	3205		TIP C	85		14.253	38.931	17.469		
MOTA	3206		TIP C	86		40.762	43.633	8.075		32.27
ATOM	3207		TIP C	87		20.139	38.471	47.202		19.79
MOTA	3208	OH2	TIP C	88		49.003	25.388	14.809		16.95
ATOM	3209	OH2	TIP C	89		48.376	21.580	21.346		26.51
MOTA	3210	OH2	TIP C	90		38.281	15.314	27.561		34.16
MOTA	3211	OH2	TIP C	91		8.631	39.984	34.095		41.37
MOTA	3212		TIP C	92		50.906	23.612	20.744		52.18
MOTA	3213		TIP C	93		53.785	20,060	24.538	1.00	24.16
ATOM	3214		TIP C	94		24.823	42.619	11.579		21.18
	3214		TIP C	95		25.075	45.083	6.146		38.65
ATOM				96		40.830	25.584	18.443		18.31
MOTA	3216		TIP C							19.16
ATOM	3217		TIP C	97		43.416	22.239	18.182		31.15
MOTA	3218		TIP C	98		13.417	34.174	40.223		19.39
MOTA	3219		TIP C	99	-	33.278	34.940	35.258		44.74
MOTA	3220	он2	TIP C	100	•	16.214	11.125	16,638	1.00	32./3

ATOM	3221	OH2	TIP C	101	53.364	20.723	14.579	1.00 34.15
ATOM	3222	OH2	TIP C	102	49.883	22.898	7.975	1.00 17.76
ATOM		OH2	TIP C	103	23.025	15.361	39.364	1.00 32.71
	3223							
ATOM	3224	OH2	TIP C	104	9.989	41.920	29.368	1.00 18.54
MOTA	3225	OH2	TIP C	105	40.434	26.276	24.857	1.00 17.36
MOTA	3226	OH2	TIP C	106	20.997	29.964	6.095	1.00 20.90
ATOM	3227	OH2		107	27.762	47.336	16.035	1.00 24.48
MOTA	3228	OH2	TIP C	108	49.284	22.771	5.126	1.00 18.73
ATOM	3229	OH2	TIP C	109	48.838	23.239	29.592	1.00 33.97
ATOM	3230	OH2	TIP C	110	28.582	23.099	35.349	1.00 20.25
MOTA	3231	OH2		111	32.528	35.162	39.110	1.00 29.39
ATOM	3232	OH2	TIP C	112	41.404	21.066	27.696	1.00 29.24
MOTA	3233	OH2	TIP C	113	41.566	30.795	24.916	1.00 29.04
	3234	OH2		114	38.888	34.349	4.634	1.00 19.24
MOTA								
MOTA	3235	OH2	TIP C	115	21.524	13.318	6.181	1.00 21.83
MOTA	3236	OH2	TIP C	116	20.262	44.365	41.166	1.00 51.68
ATOM	3237	OH2	TIP C	117	40.866	37.586	7.262	1.00 26.48
	3238	OH2	TIP C	118	24.269	19.013	20.381	1.00 20.56
MOTA								
ATOM	3239	OH2	TIP C	119	14.796	40.366	21.026	1.00 26.21
MOTA	3240	OH2	TIP C	120	40.271	21.968	24.452	1.00 22.99
ATOM	3241	OH2	TIP C	121	27.256	8.206	3.568	1.00 32.16
ATOM	3242	OH2	TIP C		38.453	23.426	21.155	1.00 20.65
ATOM	3243	OH2		123	39.489	30.192	18.787	1.00 19.64
ATOM	3244	OH2	TIP C	124	49.479	24.877	3.120	1.00 15.38
ATOM	3245	OH2	TIP C	125	23.534	17.922	36.838	1.00 21.55
ATOM	3246	OH2	TIP C	126	24.481	13.568	37.531	1.00 33.00
			TIP C		27.515	37.075	45.132	1.00 32.65
MOTA	3247	OH2						
ATOM	3248	OH2	TIP C		20.903	11.530	10.774	1.00 25.13
ATOM	3249	OH2	TIP C	129	16.996	37.117	6.834	1.00 26.72
ATOM	3250	OH2	TIP C	130	42.280	39.848	5.806	1.00 39.08
MOTA	3251	OH2	TIP C		15.426	37.238	14.643	1.00 27.36
								1.00 27.58
ATOM	3252	OH2	TIP C		47.740	29.973	16.321	
MOTA	3253	OH2	TIP C	133	52.162	19.864	18.278	1.00 19.10
ATOM	3254	OH2	TIP C	134	47.805	11.416	4.529	1.00 30.40
ATOM	3255	OH2	TIP C	135	20.920	22.905	41.964	1.00 23.80
ATOM	3256	OH2	TIP C		27.784	19.013	-1.506	1.00 28.71
							2.115	1.00 19.53
ATOM	3257	OH2		137	25.506	36.437		
MOTA	3258	OH2	TIP C		6.347	36.058	44.801	1.00 30.54
MOTA	3259	OH2	TIP C	139	18.428	23.862	8.397	1.00 19.65
ATOM	3260	OH2	TIP C	140	56.631	14.945	24.048	1.00 29.26
ATOM	3261	OH2	TIP C		36.045	33.381	-3.424	1.00 39.63
								1.00 31.49
ATOM	3262	OH2	TIP C	142	20.242	14.180	11.802	_
ATOM	3263	OH2	TIP C	143	8.614	22.301	31.526	1.00 30.94
MOTA	3264	OH2	TIP C	144	8.697	38.736	31.440	1.00 44.64
ATOM	3265	OH2	TIP C	145	21.002	20.115	40.621	1.00 23.34
ATOM	3266		TIP C		36.343	37.533	7.628	1.00 25.43
						44.970	51.125	1.00 40.01
ATOM	3267		TIP C		13.944			
MOTA	3268	OH2	TIP C	148	12.509	22.964	23.735	1.00 33.44
MOTA	3269	OH2	TIP C	149	32.555	6.398	6.686	1.00 30.50
ATOM	3270	OH2	TIP C	150	11.123	30.018	41.695	1.00 29.12
ATOM	3271		TIP C		20.406	19.454	17.419	1.00 26.72
ATOM	3272		TIP C		37.729	21.375	25.750	1.00 27.16
ATOM	3273	OH2	TIP C	153	36.922	28.170	33.507	1.00 42.28
ATOM	3274	OH2	TIP C	154	13.904	29.766	32.277	1.00 19.72
ATOM	3275		TIP C		54.556	19.732	11.775	1.00 37.67
					14.999	28.327	48.310	1.00 40.64
MOTA	3276		TIP C					
MOTA	3277		TIP C		19.001	46.759	12.106	1.00 40.48
MOTA	3278	OH2	TIP C	158	22.361	9.339	13.691	1.00 44.57
MOTA	3279	OH2	TIP C	159	26.097	16.601	36.996	1.00 27.61
ATOM	3280		TIP C		51.862	24.669	14.501	1.00 39.22
ATOM	3281		TIP C		42.713	33.316	38.299	1.00 37.21
								1.00 32.14
MOTA	3282	OH2	TIP C	102	32.074	43.316	6.583	1.00 32.14

ATOM	3283	он2 т	IP C	163	44.434	22.056	2.693	1.00 44.76
ATOM	3284	OH2 T	IP C	164	24.074	33.090	45.770	1.00 26.95
MOTA	3285			165	12.289	35.656	48.500	1.00 33.30
ATOM	3286			166	19.499	27.253	51.538	1.00 48.93
ATOM	3287			167	28.896	14.390	20.410	1.00 32.12
ATOM	3288		IP C		7.799	34.543	25.107	1.00 34.11
ATOM	3289			169	41.359	33.697	5.939	1.00 29.72
ATOM	3290			170	26.378	23.008	46.449	1.00 37.54
ATOM	3291			171	10.530	41.770	49.010	1.00 34.66
	3292			172	41.154	5.586	4.533	1.00 25.18
MOTA				173	17.462	11.487	4.521	1.00 25.18
MOTA	3293				7.600	39.527	37.113	1.00 40.32
MOTA	3294			174			37.583	1.00 30.37
ATOM	3295		IP C		3.552	23.235	40.191	1.00 36.81
ATOM	3296			176	32.818	21.891	40.191	
MOTA	3297			177	30.404	26.159		1.00 38.22 1.00 39.76
MOTA	3298			178	16.691	29.183	54.400	1.00 39.76
ATOM	3299		IP C	179	16.247	47.986	22.417	
ATOM	3300		IP C	180	37.394	44.558	11.594	1.00 39.03
MOTA	3301			181	53.552	27.209	11.822	1.00 47.97 1.00 38.41
MOTA	3302			182	10.503	32.709	12.025	
MOTA	3303		IP C	183	17.985	14.916	28.259	1.00 36.86
MOTA	3304		IP C	184	25.047	45.446	12.174	1.00 49.92
MOTA	3305		IP C	185	16.402	15.741	36.532	1.00 40.29
MOTA	3306		IP C	186	51.364	22.471	17.335	1.00 28.11
MOTA	3307		IP C	187	25.633	28.369	50.282	1.00 42.57
MOTA	3308		IP C	188	35.183	14.816	0.037	1.00 36.60
MOTA	3309		IP C	189	8.318	26.536	23.386	1.00 44.75
MOTA	3310			190	47.893	17.794	24.745	1.00 42.51
MOTA	3311			191	2.728	32.293	36.650	1.00 38.36
MOTA	3312		IP C	192	30.315	9.929	15.860	1.00 39.58
ATOM	3313			193	29.613	40.378	2.225	1.00 41.26
ATOM	3314		IP C	194	14.241	43.934	16.316	1.00 43.60
MOTA	3315	OH2 T	IP C	195	48.673	31.215	7.801	1.00 32.67
MOTA	3316	OH2 T	IP C	196	10.948	21.963	18.969	1.00 41.87
MOTA	3317	OH2 T	IP C	197	37.378	39.077	3.714	1.00 35.77
ATOM	3318	OH2 T	IP C	198	24.488	11.993	21.654	1.00 38.05
ATOM	3319	OH2 T	IP C	199	47.986	31.378	4.946	1.00 48.02
MOTA	3320	OH2 T	IP C	200	15.373	46.520	15.659	1.00 45.30
MOTA	3321	OH2 T	IP C	201	29.464	40.417	40.154	1.00 40.62
MOTA	3322	OH2 T	IP C	202	56.018	18.652	7.189	1.00 43.28
MOTA	3323	OH2 T	IP C	203	36.508	17.526	41.765	1.00 61.21
ATOM	3324	OH2 T	IP C	204	36.132	36.523	-0.637	1.00 43.56
MOTA	3325	OH2 T	IP C	205	9.832	29.974	46.230	1.00 47.33
MOTA	3326	OH2 T			12.086	37.731	18.949	1.00 44.12
MOTA	3327	OH2 T	IP C	207	4.729	26.744	22.711	1.00 40.03
ATOM	3328	OH2 T			9.555	36.540	23.357	1.00 46.94
MOTA	3329	OH2 T	IP C	209	23.046	47.732	4.343	1.00 48.13
MOTA	3330	OH2 T	IP C	210	39.932	44.592	5.460	1.00 64.51
MOTA	3331	OH2 T	IP C	211	17.996	41.071	6.267	1.00 48.35
ATOM	3332	OH2 T	IP C	212	17.866	46.493	17.139	1.00 39.09
ATOM	3333	OH2 T	IP C	213	55.520	11.908	17.658	1.00 43.06
ATOM	3334	он2 т	IP C	214	3.059	35.093	42.826	1.00 38.97
MOTA	3335	он2 т	IP C	215	31.593	14.910	43.677	1.00 44.01
MOTA	3336	он2 т			33.045	23.673	44.607	1.00 45.50
MOTA	3337	он2 т	IP C	217	42.870	35.555	7.510	1.00 29.79
ATOM	3338	OH2 T			4.112	25.648	42.564	1.00 56.65
ATOM	3339	он2 т			48.260	8.547	20.446	1.00 47.85
ATOM	3340	OH2 T			-0.925	31.171	41.173	1.00 36.99
ATOM	3341	OH2 T			41.791	22.878	0.132	1.00 56.14
ATOM	3342	OH2 T			7.088	25.685	41.540	1.00 47.43
ATOM	3343	OH2 T			24.815	4.785	13.582	1.00 47.96
ATOM	3344	OH2 T			40.690	4.520	15.174	1.00 48.76

ATOM	3345	OH2	TIP	С	225	10.029	32.425	18.562	1.00 36.30
ATOM	3346	OH2	TIP			22.346	37.737	48.941	1.00 34.15
		OH2	TIP			16.274	17.012	19.693	1.00 27.63
MOTA	3347.								
MOTA	3348	OH2	TIP	С	228	35.332	13.692	20.375	1.00 37.59
ATOM	3349	OH2	TIP	С	229	41.228	36.673	22.908	1.00 51.58
ATOM	3350	OH2				17.416	42.030	50.226	1.00 47.63
						•			
MOTA	3351		TIP			18.428	39.213	52.835	1.00 40.43
ATOM	3352	OH2	TIP	С	232	42.243	43.386	25.548	1.00 48.60
ATOM	3353	OH2	TIP	С	233	14.081	18.701	0.364	1.00 32.87
ATOM	3354	OH2	TIP		234	41.421	41.332	28.531	1.00 54.67
MOTA	3355	OH2	TIP			42.772	36.396	11.892	1.00 41.24
ATOM	3356	OH2	TIP	С	236	13.068	13.733	28.653	1.00 42.66
$ATOM \cdot$	3357 ·	OH2	TIP	C	237	10.850	26.738	7.811	1.00 40.46
ATOM	3358	OH2	TIP	C	238	16.253	20.926	45.776	1.00 44.60
ATOM	3359	OH2	TIP		239	32.681	31.139	43.220	1.00 42.20
ATOM	3360	OH2	TIP			56.267	22.254	9.280	1.00 52.44
ATOM	3361	OH2	TIP	C	241	12.553	25.304	9.942	1.00 38.77
ATOM	3362	OH2	TIP	С	242	50.727	9.516	16.775	1.00 33.38
ATOM	3363	OH2	TIP	C	243	31.871	41.347	0.512	1.00 47.78
ATOM	3364	OH2				10.008	45.092	37.807	1.00 39.52
MOTA	3365	OH2	TIP			14.551	39.030	6.708	1.00 44.26
MOTA	3366	OH2	TIP	C	246	26.955	18.903	-5.135	1.00 42.54
ATOM	3367	OH2	TIP	С	247	39.916	22.478	18.854	1.00 33.22
MOTA	3368	OH2	TIP	C	248	40.431	40.824	22.426	1.00 35.58
ATOM	3369	OH2	TIP			52.081	23.408	10.759	1.00 42.53
ATOM	3370	OH2			250	12.078	16.710	24.149	1.00 32.37
MOTA	3371	OH2				54.111	15.908	8.256	1.00 44.58
ATOM	3372	OH2	TIP	C	252	33.950	12.827	-1.753	1.00 27.02
ATOM	3373	ОН2	TIP	C	253	-0.775	26.703	40.353	1.00 43.64
ATOM	3374	OH2	TIP			1.937	33.711	40.561	1.00 42.67
MOTA	3375	OH2	TIP			8.008	24.066	18.824	1.00 51.45
MOTA	3376	OH2	TIP	С	256	11.765	27.465	3.635	1.00 47.34
ATOM	3377	OH2	TIP	C	257	27.863	43.878	9.233	1.00 32.44
MOTA	3378	он2	TIP	C	258	18.655	30.114	4.303	1.00 33.13
	3379	OH2				21.592	19.085	-3.960	1.00 39.86
ATOM									
ATOM	3380	OH2			260	41.876	24.067	25.906	1.00 26.34
MOTA	3381	OH2	TIP	С	261	46.651	10.240	2.171	1.00 44.38
MOTA	3382	OH2	TIP	C	262	32.536	15.827	32.477	1.00 43.28
MOTA	3383	он2	TIP	C	263	12.479	39.205	50.359	1.00 47.33
	3384	OH2	TIP	_	264	0.850	27.980	38.316	1.00 43.45
ATOM				-					
MOTA	3385	OH2	TIP			49.605	7.356	18.061	1.00 66.01
MOTA	3386	OH2	TIP	C	266	30.177	40.365	-3.235	1.00 44.45
ATOM	3387	OH2	TIP	C	267	39.818	12.364	0.512	1.00 48.84
ATOM	3388	OH2	TIP	C	268	38.149	44.716	27,884	1.00 51.18
		_	TIP			37.156	37.062	30.528	1.00 35.17
MOTA	3389								
MOTA	3390		TIP			51.808	7.097	12.435	1.00 51.69
ATOM	3391	OH2	TIP	C	271	54.351	12.626	12.471	1.00 47.45
MOTA	3392	OH2	TIP	C	272	50.835	31.155	13.092	1.00 55.05
ATOM	3393	OH2	TIP	C	273	12.159	35.313	52.133	1.00 52.38
ATOM	3394		TIP			21.002	44.489	13.037	1.00 39.70
ATOM	3395		TIP			37.936	23.627	34.221	1.00 48.56
MOTA	3396	OH2	TIP	C	276	45.844	30.935	31.365	1.00 43.24
ATOM	3397	OH2	TIP	C	277	38.831	48.015	15.554	1.00 49.83
ATOM	3398		TIP			5.630	28.150	44.576	1.00 48.10
ATOM	3399		TIP			8.600	24.000	45.727	1.00 49.27
ATOM	3400		TIP			54.276	20.854	7.807	1.00 36.02
MOTA	3401		TIP			3.544	34.696	46.365	1.00 43.63
ATOM	3402	OH2	TIP	C	282	24.214	46.264	46.163	1.00 48.04
MOTA	3403		TIP			7.099	32.072	19.549	1.00 54.97
MOTA	3404		TIP			36.469	22.374	41.355	1.00 52.17
									1.00 45.46
MOTA	3405		TIP			34.660	13.757	23.756	
MOTA	3406	OH2	TIP	C	286	28.516	42.981	5.402	1.00 53.58

	3405		m=n a	207	3F F30	4 000	12 012	1 00 50 07
ATOM	3407	OH2	TIP C		35.579	4.929	12.012	1.00 52.07
ATOM	3408	OH2	TIP C	288	22.974	49.682	24.299	1.00 53.67
	3409	OH2	TIP C	280	3.725	31.464	46.354	1.00 46.43
MOTA								
ATOM	3410	OH2	TIP C	290	27.340	39.594	-2.191	1.00 56.89
ATOM	3411	OH2	TIP C	291	33.413	34.856	32.335	1.00 31.78
ATOM	3412	OH2	TIP C	292	43.340	7.715	8.063	1.00 43.53
ATOM	3413	OH2	TIP C	293	28.243	21.392	-4.937	1.00 38.33
		OH2	TIP C		49.389	26.590	35.796	1.00 45.66
ATOM	3414							
MOTA	3415	OH2	TIP C	295	28.948	15.824	33.796	1.00 52.48
ATOM	3416	OH2	TIP C	296	27.347	13.383	37.207	1.00 48.27
					38.485		36.901	1.00 48.92
ATOM	3417	OH2	TIP C			26.090		
ATOM	3418	QH2	TIP C	298	12.120	20.265	11.506	1.00 50.10
ATOM	3419	OH2	TIP C	299	36.480	36.306	38.613	1.00 50.38
ATOM	3420	OH2		300	31.471	16.463	35.507	1.00 38.37
ATOM	3421	OH2	TIP C	301	42.889	5.274	2.358	1.00 33.49
	3422	он2		302	23.548	44.173	32.246	1.00 39.09
MOTA								
MOTA	3423	OH2		303	13.465	43.978	13.054	1.00 52.67
ATOM	3424	OH2	TIP C	304	25.133	43.053	4.111	1.00 52.03
					33.587	24.652	39.392	1.00 49.48
MOTA	3425	OH2		305				
ATOM	3426	OH2	TIP C	306	39.063	28.353	1.979	1.00 47.89
ATOM	3427	OH2	TIP C	307	49.357	35.834	12.150	1.00 49.22
							33.347	1.00 49.50
ATOM	3428	OH2		308	27.159	46.386		
ATOM	3429	OH2	TIP C	309	9.510	21.769	39.704	1.00 47.95
ATOM	3430	OH2	TIP C	310	34.885	32.959	39.205	1.00 51.26
			_			. —	9.747	1.00 56.02
MOTA	3431	OH2	TIP C	311	30.980	6.002		
ATOM	3432	OH2	TIP C	312	43.802	34.511	14.853	1.00 41.89
ATOM	3433	OH2	TIP C	313	36.834	4.382	5.254	1.00 39.04
					12.453	30.429	47.461	1.00 47.60
ATOM	3434	OH2	TIP C	314				
ATOM	3435	OH2	TIP C	315	39.685	40.144	30.944	1.00 54.68
ATOM	3436	OH2	TIP C	316	45.982	20.840	31.078	1.00 47.99
					32.815	36.023	42.050	1.00 45.07
ATOM	3437	OH2	TIP C					
ATOM	3438	OH2	TIP C	318	17.877	37.802	-3.699	1.00 56.30
ATOM	3439	OH2	TIP C	319	53.681	9.633	16.525	1.00 55.34
			TIP C		21.577	43.070	52.229	1.00 49.54
ATOM	3440	OH2						
ATOM	3441	OH2	TIP C	321	6.139	45.122	36.565	1.00 44.40
ATOM	3442	OH2	TIP C	322	34.695	13.561	26.782	1.00 45.99
		OH2	TIP C		17.990	33.946	-9.976	1.00 56.88
MOTA	3443							
ATOM	3444	OH2	TIP C	324	25.587	50.416	28.268	1.00 52.75
ATOM	3445	OH2	TIP C	325	27.744	42.608	42.266	1.00 44.66
	3446	OH2	TIP C		48.357	32.815	33.851	1.00 57.98
MOTA								_
ATOM	3447	OH2	TIP C	327	61.047	18.004	17.692	1.00 51.30
ATOM	3448	OH2	TIP C	328	17.327	11.069	11.972	1.00 48.28
ATOM	3449	OH2	TIP C		59.624	17.562	20.598	1.00 44.37
MOTA	3450	OH2	TIP C		40.644	39.227	19.932	1.00 37.57
MOTA	3451	OH2	TIP C	331	12.920	31.214	52.942	1.00 51.07
ATOM	3452		TIP C		37.639	0.847	19.561	1.00 49.44
MOTA	3453	OH2	TIP C	333	34.243	38.790	-3.251	1.00 54.21
ATOM	3454	OH2	TIP C	334	24.216	47.874	6.983	1.00 50.90
					15.324	34.797	6.670	1.00 45.25
ATOM	3455		TIP C					
MOTA	3456	OH2	TIP C	336	18.474	15.525	21.402	1.00 34.12
ATOM	3457	OH2	TIP C	337	40.048	8.873	26.818	1.00 49.89
					32.472	13.331	20.523	1.00 29.86
ATOM	3458	OH2						
ATOM	3459	OH2	TIP C	339	57.778	14.167	30.422	1.00 49.76
ATOM	3460	OH2			46.651	35.476	13.375	1.00 56.48
	3461	OH2			15.427	13.237	3.552	1.00 5725
ATOM					_			
MOTA	3462		TIP C		40.349	38.972	3.722	1.00 65.27
ATOM	3463	OH2	TIP C	343	8.685	28.945	15.205	1.00 59.60
ATOM	3464	OH2			11.958	41.585	22.587	1.00 37.18
								1.00 42.95
ATOM	3465	OH2			9.054	20.498	28.914	
ATOM	3466		TIP C		20.086	20.088	46.913	1.00 42.03
ATOM	3467		TIP C		40.370	35.093	2.009	1.00 49.35
ATOM	3468		TIP C		41.948	4.327	12.147	1.00 50.59
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ATOM ATOM ATOM	3469 3470 3471	OH2	TIP C TIP C TIP C	350	23.518 19.169 32.946	45.701 37.474 39.184	40.287 4.786 41.062	1.00 39.79 1.00 44.67 1.00 57.56
MOTA	3472		TIP C		37.578	47.817	18.421	1.00 51.80
MOTA	3473		TIP C		15.391	43.820	7.645	1.00 58.15
ATOM	3474		TIP C		38.205	17.257	33.401	1.00 55.84
MOTA	3475		TIP C		43.224	1.565	14.606	1.00 41.12
MOTA	3476	OH2	TIP C	356	18.704	51.623	28.487	1.00 61.11
MOTA	3477	OH2	TIP C	357	46.033	5.813	0.173	1.00 43.43
MOTA	3478	OH2	TIP C	358	51.950	27.722	14.408	1.00 45.00
ATOM	3479	OH2	TIP C	359	46.825	2.427	15.714	1.00 52.68
ATOM	3480	OH2	TIP C	360	17.624	50.111	20.315	1.00 39.65
MOTA	3481	0	нон с	361	27.534	15.877	26.687	1.00 20.00
ATOM END	3482	0	нон с	362	28.946	16.344	30.514	1.00 20.00

INTERNATIONAL SEARCH REPORT

International application No.

PCT/US01/29387

			PC1/0301/2938/			
	SSIFICATION OF SUBJECT MATTER					
IPC(7) : G01N 33/483						
US CL : 702/19						
According to International Patent Classification (IPC) or to both national classification and IPC B. FIELDS SEARCHED						
Minimum do	cumentation searched (classification system followed	l by classific	ation symbols)			
U.S. : 70	02/17, 435, 424.					
Dogumentatio	on searched other than minimum documentation to the	e extent that	t such documents are included	d in the fields searched		
Documentation	on searched other than minimum documentation to the	ic extent ma	t such documents are mender	a m the fields scalened		
						
Electronic da	ta base consulted during the international search (na	me of data b	ase and, where practicable, s	earch terms used)		
	ontinuation Sheet		•	•		
1						
G 700	UMENTS CONSIDERED TO BE RELEVANT					
		nnronrioto d	of the relevant negacine	Relevant to claim No.		
Category *	Citation of document, with indication, where a					
Y	ROSSJOHN et al. Crystal structure of the N-termir Alzheimer amyloid precursor protein. Nature Struc			1-2		
	4, pages 327-331, see entire document and especial					
	4, pages 327-331, see entire document and especial	ny page 330	in Mctious.	!		
Y	ZHANG Z. et al. Sequence-specific recognition of	the interan	alization motif of the	1-2		
1	Alzheimer's amyloid precursor protein by the X11			1-2		
	1997, Vol 16. No. 20, pages 6141-6150,		110 220 104			
	see entire document and especially page 6147.					
Y.P	MARCINKEVICIENE J. at al. Mechanism of Inhi	bition of bet	a-Site Amyloid Precursor	1		
-,-	Protein-cleaving Enzyme (BACE) by a Statine-base					
]	Chemistry. 29 June 2001, Vol 276, No. 26, pages					
i						
Y	HYNES et al. X-ray Crystal Structure of the Protes			1-2		
	Amyloid beta-Protein Precursor. Biochemistry. 199	0, Vol 29, p	ages 10018-10022,			
}	especially page 10019.					
i i						
K 2		<u></u>				
Further	documents are listed in the continuation of Box C.		See patent family annex.			
* s	pecial categories of cited documents:		later document published after the inte			
"A" document	defining the general state of the art which is not considered to be		date and not in conflict with the applic principle or theory underlying the inve			
	dar relevance					
"E" earlier ap	plication or patent published on or after the international filing date		document of particular relevance; the considered novel or cannot be consider			
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	which may throw doubts on priority claim(s) or which is cited to the publication date of another citation or other special reason (as	*Y*	document of particular relevance; the	claimed invention cannot be		
specified)		_	considered to involve an inventive step	when the document is		
"O" document	referring to an oral disclosure, use, exhibition or other means		combined with one or more other such being obvious to a person skilled in the			
1	-					
"P" document published prior to the international filing date but later than the "&"			document member of the same patent	family		
priority date claimed						
Date of the actual completion of the international search			ailing of the international sea	rch report		
18 December 2001 (18.12.2001)			TOLED	2002		
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International application No.

PCT/US01/29387

INTERNATIONAL SEARCH REPORT

tegory *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No
<u> </u>	BAILEY et al. X-ray-crystallographic studies of complexes of pepstatin A and a statine-containing human renin inhibitor with endothiapepsin. Biochem. J.1993, Vol 289, pages 363-371, especialy pages 365-366.	1-2
Y	SCHEIDIG et al. Crystal structures of bovin chymotrypsin and trypsin complexed to the inhibitor domain of Alzheimer's amyloid beta-protein precursor (APPI) and basic pancreatic trypsin inhibitor (BPTI): Engineering of inhibitors wth altered specificities. The Protein Society. September 1997, Vol 6, pages 1806-1824, see entire document and especially page 1820.	1-2
A	KOHNO et al. Thre-Dimentional Structure of the Amyloid beta Peptide (25-35) in Membrane-Mimicking Environment. Biochemistry. 1996, Vol 35, pages 16094-16104, see entire document.	1-2
A	VASSAR et al. Beta-Secretase Cleavage of Azheimer's Amyloid Precursor Protein by the Transmembrane Aspartic Protease BACE. Science. 22 October 1999, Vol 286, pages 735-741, see entire document.	1-2
A	HONG, L. et al. Structure of the Protease Domain of Memapsin 2(beta-Secretase) Complexed with Inhibitor. Science. 24 May 2000, Vol 290, No. 5489, pages 150-159, see entire document	1-2
A	SAUDER, M. et al. Modeling of substrate specifity of the Alzheimer's desease amyloid precursor protein beta-secretase. J. Mol. Biol. 2000, Vol 300, No. 2, pages 241-248, see entire document.	1-2
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INTERNATIONAL SEARCH REPORT

International application No.

PCT/US01/29387

Box I Observations where certain claims were found unsearchable (Continuation of Item 1 of first sheet)				
This international report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:				
1. Claim Nos.: because they relate to subject matter not required to be searched by this Authority, namely:				
Claim Nos.: because they relate to parts of the international application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:				
3. Claim Nos.: because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).				
Box II Observations where unity of invention is lacking (Continuation of Item 2 of first sheet)				
This International Searching Authority found multiple inventions in this international application, as follows: Please See Continuation Sheet				
1. As all required additional search fees were timely paid by the applicant, this international search report covers all searchable claims.				
2. As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.				
3. As only some of the required additional search fees were timely paid by the applicant, this international search report covers only those claims for which fees were paid, specifically claims Nos.: 1 and 2				
·				
4. No required additional search fees were timely paid by the applicant. Consequently, this international search report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:				
Remark on Protest The additional search fees were accompanied by the applicant's protest.				
No protest accompanied the payment of additional search fees.				

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International application No.

PCT/US01/29387

BOX II. OBSERVATIONS WHERE UNITY OF INVENTION IS LACKING

The inventions listed as Groups I-II do not relate to a single general inventive concept under PCT Rule 13.1 because, under PCT Rule 13.2, they lack the same or corresponding special technical features for the following reasons:

The inventions listed as Groups I-II do not relate to a single general inventive concept under PCT Rule 13.1 because, under PCT Rule 13.2, they lack the same or corresponding special technical features for the following reasons: Invention I and II are directed to different chemical and physical types regarding the critical limitations therein. For Group I, the critical feature is a crystallization of complex whereas for Group II the critical feature is the obtaining or synthesizing the agent. This application contains the following inventions or groups of inventions which are not so linked as to form a single general inventive concept under PCT Rule 13.1. In order for all inventions to be searched, the appropriate additional examination fees must be paid.

Group I, claims 1-2, drawn to crystallized complex.

Group II, claims 24 and 27 drawn to method further comprising one of the steps: obtaining and synthesizing the agen. Claims 3-23, 25,26,28-30 are directed solely to information and are therefore excluded from search.

The International Searching Authority considers that the international application does not comply with the requirements of unity of invention (Rules 13.1, 13.2 and 13.3) for reasons indicated below:

The inventions listed as Groups I-II do not relate to a single general inventive concept under PCT Rule 13.1 because, under PCT Rule 13.2, they lack the same or corresponding special technical features for the following reasons:

The inventions listed as Groups I-II do not relate to a single general inventive concept under PCT Rule 13.1 because, under PCT Rule 13.2, they lack the same or corresponding special technical features for the following reasons: Invention I and II are directed to different chemical and physical types regarding the critical limitations therein. For Group I, the critical feature is a crystallization of complex whereas for Group II the critical feature is the obtaining or synthesizing the agent.

Continuation of B. FIELDS SEARCHED Item 3:

WEST, STN, Non-patent-literature covering search terms: Cleaving Enzyme(BACE), crystallization, beta-Amyloid Precursor protein, 3-d structure of APP, Statine-based peptides.

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